~~Confidential~~

Helsinki, 16 November 2022

Addressees
Registrant(s) of Ester PSA, DEG as listed in Appendix 3 of this decision

Date of submission of the dossier subject to this decision
01/07/2021

Registered substance subject to this decision ("the Substance")
Substance name: Reaction mass of 2-{[2-(2-hydroxyethoxy)ethoxy]carbonyl}benzoic acid and 2,2'-oxydiethanol
EC number: 700-993-7

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 ***24 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. Simulation testing on ultimate degradation in surface water also requested below (triggered by Annex VIII, Section 9.2.);

2. Soil simulation testing also requested below (triggered by Annex VIII, Section 9.2.);

3. Sediment simulation testing also requested below (triggered by Annex VIII, Section 9.2.);

4. Identification of degradation products also requested below (triggered by Annex VIII, Section 9.2.);

5. Bioaccumulation in aquatic species also requested below (triggered by Annex I, Sections 0.6.1. and 4; Annex XIII, Section 2.1.);

6. Adsorption/ desorption screening (Annex VIII, Section 9.3.1.; test method: EU C.18/OECD TG 106).

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

7. Sub-chronic toxicity study (90-day) (Annex IX, Section 8.6.2.; test method: OECD TG 408) by oral route, in rats

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

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

10. Simulation testing on ultimate degradation in surface water (Annex IX, Section 9.2.1.2.; test method: EU C.25./OECD TG 309) at a temperature of 12°C. Non-extractable residues (NER) must be quantified and a scientific justification of the selected extraction procedures and solvents must be provided;

11. If result from Request 6 study are showing high adsorption potential then: 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;

12. If result from Request 6 study are showing high adsorption potential then: 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;

13. Identification of degradation products (Annex IX, 9.2.3.; test method: EU C.25./OECD TG 309 or EU C.23./OECD TG 307 or EU C.24./OECD TG 308);

14. Bioaccumulation in aquatic species (Annex IX, Section 9.3.2; test method: EU C.13./OECD TG 305, aqueous 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.

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 related to the information under Annex VIII of REACH

1. Simulation testing on ultimate degradation in surface water

1 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).

1.1. Triggering of the information requirement

2 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 (The ≥60 % pass level for the test OECD 301F only applies to mono-constituents or multi-constituents with structurally similar constituents);
  - it shows <70% degradation within 14 days in an inherent biodegradation test OECD 302 C;
- it is potentially bioaccumulative or very bioaccumulative (B/vB) as:
  - for some groups of substances (e.g. organometals, ionisable substances, surfactants) other partitioning mechanisms may drive bioaccumulation (e.g. binding to protein/cell membranes) and high potential for bioaccumulation cannot be excluded solely based on its potential to partition to lipid (LogKow);

3 As explained in Guidance on IRs and CSA Section R.11.4.2.2.2, "In cases where "not PBT/vPvB" is concluded based on results from tests with the whole substance, there should be a clear case made in the assessment for why all constituents are structurally sufficiently similar and hence also similar with regard to the PBT properties to justify such a conclusion.".

1.2. Information provided

4 Your registration dossier provides the following:

- The Substance is a multi-constituent and, as reported in IUCLID Section 1.2. it contains two main constituents (DEG and Ester PSA). These constituents differ in structure since DEG is diethylene glycol and Ester PSA is a mono ester of phthalic acid and diethylene glycol.
- Screening biodegradation data conducted with the whole substance showing the following:
  - The Substance is not readily biodegradable. The 60% degradation after 28 days in EU Method C.4-D/OECD TG 301F was determined for the whole substance, which you use to conclude that the Substance is not P/vP. In the comments to the draft decision you claim to have performed a re-assessment of the study '*triggered by the recognition that the COD value of 1.935 mg O2/mg determined during this study is approx. 25 % higher than expected*'. Based on the re-assessment you claim that '*the final degradation*

rate after 28 days is more likely to be 76% than 60% calculated from the BOD values'. You further refer to an ongoing study with the Substance, performed according to OECD TG 301F, which shows 90% degradation after 28 days. You claim the study was extended to 60 days however, the data is not reported. Overall, you have not demonstrated that the Substance is completely mineralised and you do not provide an explanation whether all constituents are structurally sufficiently similar and hence also similar with regard to the P/vP properties to justify such a conclusion. As explained above, the constituents of the Substance are structurally different and therefore the result does not provide unequivocal conclusion that all constituents would not screen P/vP;

    - the Substance is not inherently biodegradable (60% degradation after 14 days in OECD TG 302 C) so it is potentially P/vP;
- the Substance is ionisable (pKa2 =3.35 for constituent Ester PSA) and therefore high potential for bioaccumulation cannot be excluded based on available information on LogKow only.

5 In the comments of the draft decision you state that "*the monoester* [EC# 218-610-2] *is likely to be degraded to DEG and phthalate*" and since both are known to be readily degradable you conclude the Substance to be readily biodegradable. However, you do not substantiate your conclusion with supporting information. Hence you have not demonstrated that all constituents of the Substance and relevant transformation/degradation products are mineralised, i.e. screen as not P/vP.

6 Furthermore, the information in your dossier is currently incompliant and therefore it is not possible to conclude on the toxicity of the Substance (see requests 7-9 of this decision).

7 Based on the above, the available information on the Substance indicates that it is a potential PBT/vPvB substance.

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

9 The examination of the available information or adaptations, as well as the selection of the requested test and the test design are addressed in Request 10.

2. Soil simulation testing

10 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).

2.1. Triggering of the information requirement

11 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.).

12 As already explained in Request 1, the Substance is a potential PBT/vPvB substance.

13 Further, as explained in Request 11, section 11.2.1, the Substance has high potential to adsorb to soil.

14 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.

15 The examination of the available information or adaptations, as well as the conditional nature of the requirement and the selection of the requested test and the test design are addressed in Request 11.

16 In the comments to the draft decision you do not agree to perform the requested study and you provide additional information. As explained in Request 1, the issues identified in the draft decision were not fully addressed in your comments hence the request remains, as further addressed in Request 11.

3. Sediment simulation testing

17 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).

3.1. Triggering of the information requirement

18 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.).

19 As already explained in Request 1, the Substance is a potential PBT/vPvB substance.

Further, as explained in Request 11, section 11.2.1, the Substance has high potential to adsorb to sediment.

20 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.

21 The examination of the available information or adaptations, as well as the conditional nature of the requirement and the selection of the requested test and the test design are addressed in Request 12.

22 In the comments to the draft decision you do not agree to perform the requested study and you provide additional information. As explained in Request 1, the issues identified in the draft decision were not fully addressed in your comments hence the request remains, as further addressed in Request 12.

4. Identification of degradation products

23 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. Triggering of the information requirement

24 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.).

25 As already explained in Request 1, the Substance is a potential PBT/vPvB substance.

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

27 The examination of the available information or adaptations, as well as further information on the selection of the approach to generate this information are addressed in Request 13.

28 In the comments to the draft decision you do not agree to perform the requested study and you provide additional information with emphasis on the ready biodegradability potential of the Substance. You do not bring additional information with regards to the identification of degradation products. As explained in Request 1, the information provided in your comments does not fully address the issues previously identified hence the P/vP properties of the Substance remain unclear. Hence, this request remains.

5. Bioaccumulation in aquatic species

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

5.1. Triggering of the information requirement

30 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.).

31 As already explained in Request 1, the Substance is a potential PBT/vPvB substance.

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

33 The examination of the available information or adaptations, as well as the selection of the requested test and the test design are addressed in Request 14.

34 In the comments to the draft decision you do not agree to perform the requested study based on the additional information provided on degradation. As explained in Request 1, the issues identified regarding your conclusion on P/vP properties of the Substance were not fully addressed in your comments. Hence, the PBT/vPvB potential of the Substance was not clarified and the request remains.

6. Adsorption/ desorption screening

35 Adsorption/desorption screening is an information requirement under Annex VIII to REACH (Section 9.3.1).

6.1. Information provided

36 You have provided an OECD TG 121 study with the Substance.

6.2. Assessment of the information provided

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

6.2.1. The provided study does not meet the information requirement.

38 To fulfil the information requirement, a study must comply with the OECD TG 121 (Article 13(3) of REACH). Therefore, the following specifications must be met:

39 Applicability domain

a) The method is applicable to substances having a Log K_{oc} between 1.5 and 5;

40 Technical specifications impacting the sensitivity/reliability of the test

b) Duplicate determinations are conducted;
c) At least 6 reference substances are used to determine the capacity factor (k');
d) The reference substances have Log K_{oc} values which encompass the Log K_{oc} of the test material;
e) The test material and the reference substances are soluble in the mobile phase in sufficient concentration to allow their detection;
f) The regression equation used to determine the Log K_{oc} of the test material is determined at least twice daily;

41 Reporting of the methodology and results

g) The reference substances used are reported, including their purity, structural formula and CAS number;
h) Details on the fitted regression line (Log k' *versus* Log K_{oc}), including the correlation coefficient and the confidence intervals, are reported;
i) Details of the calculation of the reported Log K_{oc} are provided.

42 Your registration dossier provides an OECD TG 121 study showing the following:

43 Applicability domain

a) The Substance has a Log K_{oc} -0.7, thus it is out of applicability domain;

44 Technical specifications impacting the sensitivity/reliability of the test

b) Duplicate determinations were not conducted;
c) The number of reference substances used to determine the capacity factor (k') was not specified;
d) The log K_{oc} values of the reference substances were not specified;
e) The solubility of the reference substances in the mobile phase was not specified;
f) The regression equation used to determine the Log K_{oc} of the test material was not determined at least twice daily. The frequency was not specified;

45 Reporting of the methodology and results

g) The reference substances used are not reported, including their purity, structural formula and CAS number;
h) Details on the fitted regression line (Log k' *versus* Log K_{oc}), including the correlation coefficient and the confidence intervals, are not reported;
i) Details of the calculation of the reported Log K_{oc} are not provided.

46 Based on the above, there are critical methodological deficiencies resulting in the rejection of the study results since the Substance is outside the applicability domain of the OECD TG 121. Furthermore, the reporting of the study is not sufficient to conduct an independent assessment of its reliability.

47 Therefore, the requirements of the OECD TG 121 are not met.

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

6.3. Study design and test specifications

49 An OECD TG 106 Batch Equilibrium Method is the appropriate method to study the adsorption of the Substance. This method uses a range of actual soils and so represents a more realistic scenario than the HPLC (OECD 121) method. The ionisable properties of the Substance should be considered when selecting the appropriate test design. For ionisable substances, soil types should cover a wide range of pH.

Reasons related to the information under Annex IX of REACH

7. Sub-chronic toxicity study (90-day)

50 A sub-chronic toxicity study (90 day) is an information requirement under Annex IX, Section 8.6.2.

7.1. Information provided

51 You have provided a justification for waiving the 90-day study: "*In accordance with section 1 of REACH Annex XI, a subchronic repeated dose toxicity study (OECD TG 413) is not required if relevant data are available to assess the risk of repeated uptake*.. Further, you refer to available data on "*acute oral and dermal (*[redacted]*, 2012) and subacute (4-week) oral toxicity studies (*[redacted]*, 2013) in rats",* lack of acute and repeated dose toxicity classification, and state that "*A qualitative and quantitative evaluation of the toxicological properties of the substance indicates that while a study with longer exposure duration might lead to a starting point for estimation of DNELs different from the subacute study it would not generally change the hazard characterization"*. Based on this you conclude that "*in view of the limited additional knowledge that data from a longer term exposure study would provide to improve the current risk and hazard characterization of the substance and the need to consider animal welfare, a subchronic repeated dose toxicity study has no priority"*.

7.2. Assessment of the information provided

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

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

53 A registrant may only adapt this information requirement based on either the general rules set out in Annex XI or the specific rules of Column 2, Annex IX, Section 8.6.2. As summarized above, you unspecifically refer to an adaptation of this information requirement in accordance with Annex XI, section 1. However, your justification to omit the study cannot be related to any legal ground for adaptation under Annex XI to REACH or under the specific rules of Column 2, Annex IX, Section 8.6.2.

54 Therefore, your adaptation is rejected.

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

7.3. Specification of the study design

56 Following the criteria provided in Annex IX, Section 8.6.2, Column 2, the oral route is the most appropriate route of administration to investigate repeated dose toxicity of the Substance; Guidance on IRs and CSA, Section R.7.5.6.3.2.

57 According to the OECD TG 408, the rat is the preferred species.

58 Therefore, the study must be performed in rats according to the OECD TG 408 with oral administration of the Substance.

8. Long-term toxicity testing on aquatic invertebrates

59 Long-term toxicity testing on aquatic invertebrates is an information requirement under Annex IX to REACH (Section 9.1.5.).

8.1. Information provided

60 You have adapted this information requirement by using Column 2 of Annex IX, Section 9.1. To support the adaptation, you have provided following justification:

(i) "In accordance with REACH Regulation, Annex IX, column 2, the study does not need to be conducted as the chemical safety assessment indicates no need. The substance is water soluble in each ratio and the study for acute toxicity showed no effect up to the hightest test concentration of 100 mg/L."

8.2. Assessment of the information provided

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

8.2.1. Annex IX, Section 9.1., Column 2 is not a valid basis to omit the study

62 Annex IX, Section 9.1., Column 2 does not allow omitting the need to submit information on long-term toxicity to aquatic invertebrates under Column 1. It must be understood as a trigger for providing further information on aquatic invertebrates if the chemical safety assessment according to Annex I indicates the need (Decision of the Board of Appeal in case A-011-2018).

63 Your adaptation is therefore rejected.

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

8.3. Study design and test specifications

65 The Substance is difficult to test due to the adsorptive properties (the substance is ionisable, pKa2 =3.35 for constituent Ester PSA). OECD TG 211 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 211. 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.

9. Long-term toxicity testing on fish

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

9.1. Information provided

67 You have adapted this information requirement by using Column 2 of Annex IX, Section 9.1. To support the adaptation provided in your dossier, you have provided following justification:

(i) "In accordance with REACH Regulation, Annex IX, column 2, the study does not need to be conducted as the chemical safety assessment indicates no need. The substance is water soluble in each ratio and the study for acute toxicity showed no effect up to the hightest test concentration of 100 mg/L."

In the comments to the draft decision you bring forward several additional considerations to omit the study: Firstly, you consider that the request should be suspended until the decision of the General Court on appeal case T-655/20, which challenges the BoA decision A-010-2018. You further refer to animal welfare reasons by referring to Para. 132 of C-471/18 P stating that *"It follows from those general provisions, which are to be construed in the light of recital 47 of the REACH Regulation, according to which it is necessary to replace, reduce or refine testing on vertebrate animals', that a registrant has, generally and therefore especially where ECHA issues it with a decision asking it to complete its registration dossier with a study involving animal testing, not simply the possibility but the obligation to generate information obtained by means other than animal testing 'whenever possible' and to undertake such testing 'only as a last resort'."*

Finally, you provide further arguments supporting no need for long-term testing on fish. Specifically, you claim that the Substance is: a) not acutely toxic; b) poorly water soluble; c) readily biodegradable; and d) has all PEC/PNEC values below 1. Furthermore, you remark that, if the request persists, you will consider the need for further vertebrate testing after evaluation of the results of the long-term toxicity testing on aquatic invertebrates requested in Request 8 of this decision.

9.2. Assessment of the information provided

68 We have assessed the information provided in your dossier and identified the following issue:

9.2.1. Annex IX, Section 9.1., Column 2 is not a valid basis to omit the study

69 Annex IX, Section 9.1., Column 2 does not allow omitting the need to submit information on long-term toxicity to fish under Column 1. It must be understood as a trigger for providing further information on long-term toxicity to fish if the chemical safety assessment according to Annex I indicates the need (Decision of the Board of Appeal in case A-011-2018).

70 We have assessed the information provided in your comments to the draft decision and identified the following issues:

9.2.2. Ongoing court proceedings

71 ECHA notes that acts and decisions of EU Institutions and agencies are presumed lawful until they are declared void by the EU Courts. Therefore, while the court proceedings you are referring to in your comments are pending, the relevant findings of the Board of Appeal as set out above remain fully applicable.

9.2.3. *Animal welfare*

72 A registrant may only adapt this information requirement based on the general rules set out in Annex XI. ECHA remarks that minimisation of vertebrate animal testing is not on its own a legal ground for adaptation under the general rules of Annex XI.

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

73 Finally, a registrant may only adapt this information requirement based on the general rules set out in Annex XI. You refer to several properties of the Substance (i.e. solubility, biodegradability, low acute toxicity) and to safety assessment (i.e. PEC/PNEC values and results of chronic data on aquatic invertebrates) to justify not providing the requested study. However, you do not refer to any legal ground for adaptation under Annex XI to REACH. Hence, you have not demonstrated that this information can be omitted.

74 Your adaptation provided in the dossier and the additional arguments brought up in your comments are therefore rejected.

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

9.3. Study design and test specifications

76 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.).

77 The OECD TG 210 specifies that, for difficult to test substances, the 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 and test specifications' under Request 8.

10. Simulation testing on ultimate degradation in surface water

78 Simulation testing on ultimate degradation in surface water (Annex IX, Section 9.2.1.2) is a standard information requirement in Annex IX to REACH.

10.1. Information provided

79 ECHA understands that you have adapted this standard information requirement by applying weight of evidence (WoE) adaptation in accordance with Annex XI, section 1.2. To support the adaptation, you have provided the following information with the Substance:

(i) QSAR prediction with EAWAG-BDD model (2021)

(ii) EU Method C.4-D/OECD TG 301F study (2011)

(iii) OECD 302C study (2012)

80 You conclude that "The combination of the outcome of the EAWAG model, which is included in its successor envipath, with the biodegradation behavior in screening tests of [the Substance] strongly suggests a high potential for biodegradation in sediment and surface water as well".

10.2. Assessment of the information provided

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

82 Annex XI, Section 1.2 states that there may be sufficient weight of evidence from several independent sources of information enabling, through a reasoned justification, a conclusion on the information requirement, while the information from each single source alone is insufficient to fulfil the information requirement.

83 The justification must have regard to the information that would otherwise be obtained from the study that must normally be performed for this information requirement.

84 According to Guidance on IRs and CSA R.4, a weight of evidence adaptation involves an assessment of the relative values/weights of the different sources of information submitted. The weight given is based on the reliability of the data, consistency of results/data, nature and severity of effects, and relevance and coverage of the information for the given regulatory information requirement. Subsequently, relevance, reliability, coverage, consistency and results of these sources of information must be balanced in order to decide whether they together provide sufficient weight to conclude on the corresponding information requirement.

85 Relevant information that can be used to support weight of evidence adaptation for the information requirement of Annex IX, Section 9.2.1.2 includes similar information that is produced by the OECD TG 309. OECD TG 309 requires the study to investigate the following key elements:

1. the rate of aerobic transformation of the test material in natural surface water is determined

2. the identity and rates of formation and decline of transformation/degradation products are determined if those are:

   a. detected at ≥ 10% of the applied radioactivity (AR) in the total water-sediment system at any sampling time, or

   b. continuously increasing during the study even if their concentrations are < 10% AR (unless appropriate justification is provided).

Concerning key element (1):

86 Study (i) provides information on the probability of biodegradation, which does not correspond to the aerobic transformation rate in natural surface water.

87 Study (ii) investigate the ultimate aerobic biodegradation (as measured by oxygen uptake) of the test material under low inoculum (activated sludge) concentration, which does not correspond to the aerobic transformation rate in natural surface water.

88 Study (iii) investigates the ultimate aerobic biodegradation (as measured by oxygen uptake) of the test material under high inoculum (activated sludge) concentration, which does not correspond to the aerobic transformation rate in natural surface water.

Concerning key element (2):

89 Studies (ii-iii) do not provide any information on the identity and rates of formation and decline of transformation/degradation products.

90 Study (i) may provide relevant information on the identity of transformation/degradation products. However, the reliability of this source of information is significantly affected by the deficiencies explained in Request 13.

91 Taken together, none of the sources of information provide relevant information on the rate of aerobic transformation of the test material in natural surface water. The only source of information that provides relevant information on identity of transformation/degradation products is source of information (i), but the information is not reliable as explained above.

92 It is therefore not possible to conclude, based on any source of information alone or considered together, whether the Substance has or has not the particular properties foreseen to be investigated in a study conducted according to the OECD TG 309. Therefore, your adaptation is rejected.

93 In your comments to the draft decision you do not agree to perform the requested test. Instead, you propose to adapt this information requirement based on Annex IX, section 9.2.1.2., column 2 since the Substance is considered readily biodegradable. In support of your adaptation you refer to the screening studies (i.e. two tests performed according to OECD TG 301 F and one performed according to OECD TG 302 C).

94 Under Section 9.2.1.2., Column 2 of Annex IX to REACH, this information requirement may be omitted if the substance is readily biodegradable.

95 As explained in Request 1, you have not demonstrated that all constituents of the Substance are readily biodegradable hence, the Substance is screening as potentially P/vP and further testing is required. Therefore, your adaptation is rejected. On this basis, the information requirement is not fulfilled.

10.3. Study design and test specifications

96 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.

97 You must perform the test, by following the pelagic test option with natural surface water containing approximately 15 mg dw/L of suspended solids (acceptable concentration between 10 and 20 mg dw/L) (Guidance on IRs and CSA, Section R.11.4.1.1.3.).

98 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 309.

99 As specified in Guidance on IRs and CSA, Section R.7.9.4.1., the organic carbon (OC) concentration in surface water simulation tests is typically 2 to 3 orders of magnitude higher than the test material concentration and the formation of non-extractable residues (NERs) may be significant in surface water tests. Therefore, non-extractable residues (NER) must be quantified. The reporting of results must include a scientific justification of the used extraction procedures and solvents. By default, total NER is regarded as non-degraded Substance. However, if reasonably justified and analytically demonstrated a certain part of NER may be differentiated and quantified as irreversibly bound or as degraded to biogenic NER, such fractions could be regarded as removed when calculating the degradation half-life(s) (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.

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

11. Soil simulation testing

101 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.

11.1. Information provided

102 ECHA understands that you consider that soil simulation testing is not required since the Substance has no high potential for adsorption to soil. You have provided the following justification: "An experimental study on the adsorption/desorption behavior of the substance was performed ([redacted] 2013) yielding a log Koc of -0.7, rendering the substance not adsorptive. Therefore, accumulation in the terrestrial compartment is not expected."

103 Furthermore, ECHA understands that you have adapted this standard information requirement by applying a weight of evidence (WoE) adaptation in accordance with Annex XI, section 1.2. To support the adaptation, you have provided the following information with the Substance:

(i) QSAR prediction with EAWAG-BDD model, 2021

(ii) EU Method C.4-D/OECD TG 301F study (2011)

(iii) OECD 302 C study (2012)

104 You conclude that "The combination of the outcome of the EAWAG model, which is included in its successor envipath, with the biodegradation behavior in screening tests of the [Substance] strongly suggests a high potential for ultimate biodegradation in soil."

11.2. Assessment of the information provided

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

11.2.1. The Substance is adsorptive

106 As explained above, soil simulation testing is required for substances with a high potential for adsorption (Section 9.2.1.3 of Annex IX).

107 You indicate that the Substance has low adsorption potential based on the Log Koc of -0.7 measured in the submitted OECD TG 121 study.

108 As explained in Request 6, the information provided on adsorption/desorption is not reliable, therefore the provided Log Koc results cannot be used to conclude that the Substance is not adsorptive.

109 ECHA notes that the Substance is ionisable (pKa2 =3.35 for constituent Ester PSA). Ionisable substances have high potential to adsorb to soil and sediment since they bind to substrates of opposite charge (e.g. cationically charged substances bind to negatively charged humic acids, clay, microorganisms etc; anionic compounds bind to positively charged Si, Al or Fe oxides) (Guidance on IRs and CSA, Table R.7.8-2).

110 Therefore, in the absence of results from an appropriate batch equilibrium test (OECD TG 106) using relevant soil and/or sediment samples demonstrating that Log Koc <4[2], the Substance is considered as adsorptive since ionisable.

111 As a consequence, the information on simulation testing of ultimate degradation in soil is required.

11.2.2. Weight of evidence adaptation

112 Annex XI, Section 1.2 states that there may be sufficient weight of evidence from several independent sources of information enabling, through a reasoned justification, a conclusion

[2] https://echa.europa.eu/standard-information-requirements-recommendations

on the information requirement, while the information from each single source alone is insufficient to fulfil the information requirement.

113 The justification must have regard to the information that would otherwise be obtained from the study that must normally be performed for this information requirement.

114 According to Guidance on IRs and CSA, Section R.4, a weight of evidence adaptation involves an assessment of the relative values/weights of the different sources of information submitted. The weight given is based on the reliability of the data, consistency of results/data, nature and severity of effects, and relevance and coverage of the information for the given regulatory information requirement. Subsequently, relevance, reliability, coverage, consistency and results of these sources of information must be balanced in order to decide whether they together provide sufficient weight to conclude on the corresponding information requirement.

115 Relevant information that can be used to support weight of evidence adaptation for the information requirement of Annex IX, Section 9.2.1.3 includes similar information that is produced by the OECD TG 307. OECD TG 307 requires the study to investigate the following key elements:

1. the rate of aerobic and anaerobic transformation of the test material in four soil types, and

2. the identity and rates of formation and decline of transformation products in at least one soil type

116 Concerning key element (1):

117 Study (i) provides information on the probability of biodegradation, which does not correspond to the rate of aerobic and anaerobic transformation of the test material in four soil types.

118 Study (ii) investigates the ultimate aerobic biodegradation (as measured by oxygen uptake) of the test material under low inoculum (activated sludge) concentration, which does not correspond to the rate of aerobic and anaerobic transformation of the test material in four soil types.

119 Study (iii) investigates the ultimate aerobic biodegradation (as measured by oxygen uptake) of the test material under high inoculum (activated sludge) concentration, which does not correspond to the rate of aerobic and anaerobic transformation of the test material in four soil types.

120 Concerning key element (2):

121 Studies (ii-iii) do not provide any information on the identity and rates of formation and decline of transformation/degradation products.

122 Study (i) may provide relevant information on the identity of transformation/degradation products. However, the reliability of this source of information is significantly affected by the deficiencies explained in Request 13.

123 Taken together, none of the sources of information provide relevant information on the rate of aerobic and anaerobic transformation of the test material in four soil types. The only source of information that provides relevant information on identity of transformation/degradation products is source of information (i), but the information is not reliable as explained above.

124 It is therefore not possible to conclude, based on any source of information alone or considered together, whether the Substance has or has not the particular properties

foreseen to be investigated in a study conducted according to the OECD TG 307. Therefore, your adaptation is rejected.

125 In your comments to the draft decision you do not agree to perform the requested test. Instead, you propose to adapt this information requirement based on Annex IX, section 9.2.1.3., column 2 since the Substance is considered readily biodegradable. In support of your adaptation you refer to the screening studies (i.e. two tests performed according to OECD TG 301 F and one performed according to OECD TG 302 C).

126 Under Section 9.2.1.3., Column 2 of Annex IX to REACH, this information requirement may be omitted if the substance is readily biodegradable.

127 As explained in Request 1, you have not demonstrated that all constituents of the Substance are readily biodegradable hence, the Substance is screening as potentially P/vP and further testing is required. Therefore, your adaptation is rejected.

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

11.3. Conditional nature of the requirements

129 The request for soil simulation testing is dependent on the result of Request 6. In that respect, as explained under Request 6, your dossier currently does not include a reliable value on the adsorption coefficient of the Substance. However, as explained above under section 11.2.1, based on the information currently contained in the dossier, the Substance may be highly adsorptive.

130 In case the Substance or any of its consituents prove to be be highly adsorptive (*i.e.* Log Koc > 4) then soil simulation testing is required.

131 Therefore, soil simulation testing must only be conducted if the data generated under Request 6 demonstrate that the Substance and/or its constituents are adsorptive (*i.e.* Log Koc > 4). The deadline set by this decision allows for the sequential testing, where necessary.

11.4. Study design and test specifications

132 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.

133 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).

134 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 309.

135 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.

136 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.).

12. Sediment simulation testing

137 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.

138 The Substance is ionisable and for the reasons explained in Request 11 (section 11.2.1), it has high potential for adsorption to sediment.

12.1. Information provided

139 ECHA understands that you have adapted this standard information requirement by applying weight of evidence (WoE) adaptation in accordance with Annex XI, section 1.2. To support the adaptation, you have provided the following information with the Substance:

(i) QSAR prediction with EAWAG-BDD model (2021)

(ii) EU Method C.4-D/OECD TG 301F study (2011)

(iii) OECD 302C study (2012)

140 You conclude that "The combination of the outcome of the EAWAG model, which is included in its successor envipath, with the biodegradation behavior in screening tests of [the Substance] strongly suggests a high potential for biodegradation in sediment and surface water as well".

12.2. Assessment of the information provided

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

142 Annex XI, Section 1.2 states that there may be sufficient weight of evidence from several independent sources of information enabling, through a reasoned justification, a conclusion on the information requirement, while the information from each single source alone is insufficient to fulfil the information requirement.

143 The justification must have regard to the information that would otherwise be obtained from the study that must normally be performed for this information requirement.

144 According to Guidance on IRs and CSA R.4, a weight of evidence adaptation involves an assessment of the relative values/weights of the different sources of information submitted. The weight given is based on the reliability of the data, consistency of results/data, nature and severity of effects, and relevance and coverage of the information for the given regulatory information requirement. Subsequently, relevance, reliability, coverage, consistency and results of these sources of information must be balanced in order to decide whether they together provide sufficient weight to conclude on the corresponding information requirement.

145 Relevant information that can be used to support weight of evidence adaptation for the information requirement of Annex IX, Section 9.2.1.4 includes similar information that is produced by the OECD TG 308. OECD TG 308 requires the study to investigate the following key elements:

1. the rate of aerobic and/or anaerobic transformation of the test material on at least two sediments, and
2. the identity and rates of formation and decline of transformation products;

146 Concerning key element (1):

147 Study (i) provides information on the probability of biodegradation, which does not correspond to the aerobic and/or anaerobic transformation rate in at least two sediments.

148 Study (ii) investigate the ultimate aerobic biodegradation (as measured by oxygen uptake) of the test material under low inoculum (activated sludge) concentration, which does not correspond to the aerobic and/or anaerobic transformation rate in at least two sediments.

149 Study (iii) investigates the ultimate aerobic biodegradation (as measured by oxygen uptake) of the test material under high inoculum (activated sludge) concentration, which does not correspond to the aerobic and/or anaerobic transformation rate in at least two sediments.

150 Concerning key element (2):

151 Studies (ii-iii) do not provide any information on the identity and rates of formation and decline of transformation/degradation products.

152 Study (i) may provide relevant information on the identity of transformation/degradation products. However, the reliability of this source of information is significantly affected by the deficiencies explained in Request 13.

153 Taken together, none of the sources of information provide relevant information on the the aerobic and/or anaerobic transformation rate in at least two sediments. The only source of information that provides relevant information on identity of transformation/degradation products is source of information (i), but the information is not reliable as explained above.

154 It is therefore not possible to conclude, based on any source of information alone or considered together, whether the Substance has or has not the particular properties foreseen to be investigated in a study conducted according to the OECD TG 308. Therefore, your adaptation is rejected.

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

156 In your comments to the draft decision you do not agree to perform the requested test. Instead, you propose to adapt this information requirement based on Annex IX, section 9.2.1.4., column 2 since the Substance is considered readily biodegradable. In support of your adaptation you refer to the screening studies (i.e. two tests performed according to OECD TG 301 F and one performed according to OECD TG 302 C).

157 Under Section 9.2.1.4., Column 2 of Annex IX to REACH, this information requirement may be omitted if the substance is readily biodegradable.

158 As explained in Request 1, you have not demonstrated that all constituents of the Substance are readily biodegradable hence, the Substance is screening as potentially P/vP and further testing is required. Therefore, your adaptation is rejected.

12.3. Conditional nature of the requirements

159 The request for sediment simulation testing is dependent on the result of Request 6. In that respect, as explained under Request 6, your dossier currently does not include a reliable

value on the adsorption coefficient of the Substance. However, as explained above under section 11.2.1, based on the information currently contained in the dossier, the Substance may be highly adsorptive.

160 In case the Substance or any of its consituents prove to be be highly adsorptive (*i.e.* Log Koc > 4) then sediment simulation testing is required.

161 Therefore, sediment simulation testing must only be conducted if the data generated under Request 6 demonstrate that the Substance and/or its constituents are adsorptive (*i.e.* Log Koc > 4). The deadline set by this decision allows for the sequential testing, where necessary.

12.4. Study design and test specifications

162 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.

163 In accordance with the specifications of the 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.

164 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

165 In accordance with the specifications of the 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.

166 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.).

13. Identification of degradation products

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

13.1. Information provided

168 You have adapted this information requirement by using Qualitative or Quantitative Structure-Activity Relationships ((Q)SARs). To support the adaptation, you have provided following information a QSAR prediction with EAWAG-BDD model (2021).

13.2. Assessment of the information provided

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

13.2.1. Assessment of (Q)SAR information

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

i. the prediction needs to be derived from a scientifically valid model,

ii. the substance must fall within the applicability domain of the model,

iii. results need to be adequate for the purpose of risk assessment or classification and labelling, and

iv. adequate and reliable documentation of the method must be provided.

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

13.2.1.1. The prediction is not adequate due to low reliability

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

- the model predicts well substances that are similar to the substance of interest.

173 You identified biodegradation products by estimating two biodegradation steps for a representative structure of the Substance (Ester PSA) with EAWAG-BBD model.

174 In the model documentation you have provided, you have not indicated whether there are similar substances from the training set of the model.

175 In the absence of this information, you have not not demonstrated that the model predicts well substances that are similar to the Substance. Therefore, it is not possible to assess the correctness of the EAWAG method in predicting the biodegradation pathway for the Substance.

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

177 Based on the above, your adaptation is rejected.

178 In your comments to the draft decision you do not agree to perform the requested test. Instead, you propose to adapt this information requirement based on Annex IX, section 9.2.3., column 2 since the Substance is considered readily biodegradable. In support of your adaptation you refer to the screening studies (i.e. two tests performed according to OECD TG 301 F and one performed according to OECD TG 302 C).

179 Under Section 9.2.3., Column 2 of Annex IX to REACH, this information requirement may be omitted if the substance is readily biodegradable.

180 As explained in Request 1, you have not demonstrated that all constituents of the Substance are readily biodegradable hence, the Substance is screening as potentially P/vP and further testing is required. Therefore, your adaptation is rejected.

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

13.3. Study design and test specifications

182 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 must obtain this information from one of the degradation studies requested in Requests 10, 11 or 12 .

183 To determine the degradation rate of the Substance, the requested study according to the OECD TG 309 (Request 10) must be conducted at 12°C and at a test concentration < 100 µg/L. However, to overcome potential analytical limitations with the identification and quantification of major transformation/degradation products, you may consider running a parallel test at higher temperature (but within the frame provided by the test guideline, e.g. 20°C) and at higher application rate (i.e. > 100 µg/L).

184 To determine the degradation rate of the Substance, the requested studies according to the OECD TG 308/307 (Requests 11 and 12) 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).

14. Bioaccumulation in aquatic species

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

14.1. Information provided

186 You have adapted this information requirement by using Column 2 of Annex IX, Section 9.3.2. To support the adaptation, you have provided the following information:

(i) the study does not need to be conducted because the substance has a low potential for bioaccumulation based on Log Kow <=3. The Substance has low potential for bioaccumulation based on a weighted Log Kow of 1.0 (range 0.9 – 1.9);

14.2. Assessment of information provided

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

14.2.1. The Log Kow is not a valid descriptor of the bioaccumulation potential of the Substance

188 Under Section 9.3.2., Column 2, first indent of Annex IX to REACH, the study may be omitted if the substance has a low potential for bioaccumulation and/or a low potential to cross biological membranes.

189 A low Log Kow (i.e. Log Kow < 3) on its own may be used to show low potential for bioaccumulation only if the potential for bioaccumulation of the substance is solely driven

by lipophilicity. This excludes, for example, situations where the substance is surface active or ionisable at environmental pH (pH 4 – 9).

190 Your registration dossier provides an adaptation stating that the log Kow is < 3 without further explanation.

191 However, the Substance is ionisable at environmental pH (pKa2 =3.35 for constituent Ester PSA).

192 Therefore, the Log Kow is not a valid descriptor of the bioaccumulation potential of the Substance and your adaptation is rejected.

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

14.3. Study design and test specifications

194 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.

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

196 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.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 18 October 2021.

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

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

ECHA notified the draft decision to the competent authorities of the Member States for proposals for amendment.

As no amendments were proposed, ECHA adopted the decision under Article 51(3) of REACH.

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.

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[3].

(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 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.

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

Technical instructions on how to report the above is available in the manual on How to prepare registration and PPORD dossiers[4].

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.

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