Helsinki, 15 November 2022

Addressee
Registrant of 6-(1-phenylethyl)-1,2,3,4-tetrahydronaphthalene listed in the last Appendix of this decision

Registered substance subject to this decision (the Substance)
Substance name: 6-(1-phenylethyl)-1,2,3,4-tetrahydronaphthalene
EC/List number: 400-370-7

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

DECISION ON SUBSTANCE EVALUATION

Under Article 46 of Regulation (EC) No 1907/2006 (REACH), you must submit the information listed below:

A. Information required to clarify the potential risk related to PBT/vPvB

1. Partition Coefficient (1-Octanol/Water): Slow-Stirring Method (test method: OECD TG 123) or HPLC method (test method: OECD TG 117), with the constituents of the Substance specified in the table below:

	Constituents	EC / List no.	CAS RN
1	[redacted]	-	[redacted]
2	[redacted]	-	[redacted]
3	[redacted]	-	[redacted]
4	[redacted]	-	[redacted]
5	[redacted]	[redacted]	[redacted]

- The constituents must be tested separately.
- If the HPLC method (OECD TG 117) is selected, the reference substances must be aromatic hydrocarbons having well-established log Kow values and the highest log Kow value for the reference substances must be ≥ 6.5.

Deadline

The information must be submitted by **22 November 2023**.

Conditions to comply with the information requested

To comply with this decision, you must submit the information in an updated registration dossier, by the deadline indicated above. The information must comply with the IUCLID robust study summary format. You must also attach the full study report for the corresponding studies in the corresponding endpoint of IUCLID.

You must update the chemical safety report, where relevant, including any changes to classification and labelling, based on the newly generated information.

You will find the justifications for the requests in this decision in the Appendix A entitled ''Reasons to request information to clarify the potential risk'.

You will find the procedural steps followed to reach the adopted decision and some technical guidance detailed in further Appendices.

Appeal

This decision 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.

[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.

Basis for substance evaluation

The objective of substance evaluation under REACH is to allow for the generation of further information on substances suspected of posing a risk to human health or the environment ('potential risk').

ECHA has concluded that further information on the Substance is necessary to enable the evaluating Member State Competent Authority (MSCA) to clarify a potential risk and whether regulatory risk management is required to ensure the safe use of the Substance.

The ECHA decision requesting further information is based on the following:

(1) There is a potential risk to human health or the environment, based on a combination of hazard and exposure information;
(2) Information is necessary to clarify the potential risk identified; and
(3) There is a realistic possibility that the information requested would allow improved risk management measures to be taken.

The Appendices entitled 'Reasons to request information' describe why the requested information are necessary and appropriate.

Appendix A – Reasons to request information to clarify the potential risk related to PBT/vPvB properties

1. Potential risk

1.1 Potential hazard of the Substance

Following its assessment of the available relevant information on the Substance, the evaluating MSCA and ECHA have identified the following potential hazard(s) which must be clarified.

a) Potential P/vP properties of the Substance

If a substance fulfils the criteria in Section 1.1.1 or 1.2.1 of Annex XIII to REACH, it is considered that it has persistent (P) or very persistent (vP) properties.

For the purpose of the P/vP assessment and to check whether the criteria are fulfilled, the information listed in Section 3.2.1 to Annex XIII, including results from simulation tests, must be considered.

If no such data are available, it is necessary to consider the screening information of Section 3.1.1 to Annex XIII, such as screening tests and QSAR predictions.

The available information suggests that the Substance may have P/vP properties, as described below.

Evidence based on experimental data

No experimental data is available for abiotic degradation for the Substance or its constituents. However, hydrolysis is not expected to be a relevant degradation pathway based on the lack of hydrolysable functional groups in the constituents.

- You have submitted a modified OECD TG 301B study on the Substance. The study is GLP compliant. The test material was ^{14}C-radiolabelled [redacted], reported to be uniformly labelled on both aromatic rings. The structure reported is for [redacted] (constituent 1). It is not indicated whether also other constituents were radiolabelled or only constituent 1.

  The test concentration was [redacted] µg/L. The study report states that modification of the standard test procedure was considered necessary because of the low water solubility of the test material (~70 µg/L). The inoculum was from a municipal wastewater treatment plant (inoculum concentration: mixed liquor suspended solids (MLSS) [redacted] mg/L). The inoculum to test substance ratio was 600 mg/mg whereas according to OECD TG 301B, the maximum ratio permitted would be 3 mg/mg, based on inoculum concentration of 30 mg/L and test concentration of 10 mg TOC/L (assuming C content of main constituent equals to the C content of whole test material). Mineralisation was 6% during 28 days.

  The decrease in ^{14}C-labelled test item concentration was 95% in viable test and 36% in sterile control during 28 days. 57 to 67% of the initial ^{14}C-label were recovered as water soluble transformation products in the viable test at the end of the study. At the conclusion of the study, the recovery of the radioactivity ranged from 62 to 79% for both the viable test and sterile controls. Different extraction procedures did not increase the recovery and it was suggested that some ^{14}C-labelled test material may have been lost by volatilisation. Most radioactivity remaining in the viable test was reported to

consist of water soluble ^{14}C-degradation products which were not identified. The study is indicated as a ready biodegradability study in the dossier.

ECHA notes that according to the OECD TG 301B, this test is suitable for poorly soluble substances and the test concentration should be 10-20 mg DOC/L. ECHA guidance R.7b (ECHA 2017c) indicates that "*where possible a lower test substance concentration than is generally recommended by the test guideline/method should still allow the assessment of biodegradability to be determined reliably through the measurement of carbon dioxide evolution, oxygen demand or dissolved organic carbon removal.*" Therefore, ECHA considers that the study can be used for the assessment despite the low concentration. However, the guidance also states that ready biodegradability tests are "*stringent screening tests, conducted under aerobic conditions, in which a high concentration of the test substance (in the range of 2 to 100 mg/L) is used*". Therefore, the study is not equivalent to a ready biodegrability test due to the low test concentration and the high inoculum to test substance ratio.

As the conditions were more favourable for biodegradation than in a standard ready biodegradability test, and as the pass level for ready biodegradation was still not reached, ECHA considers that in a standard ready biodegradability study the percentage degradation would most likely not be higher than in this study. Therefore, despite the deviations from the test guideline, ECHA considers that this study indicates that the test material is not readily biodegradable and that it is potentially P or vP.

Considering the high concentration of constituent 1 and the low mineralisation, it can be concluded that constituent 1 is not readily biodegradable and that it is potentially P or vP. The significant primary degradation together with the low mineralisation suggest that constituent 1 underwent significant primary degradation into unidentified transformation products, which are potentially P or vP. For the other constituents, no conclusions can be drawn based on this study due to their low concentrations.

- You have submitted a modified OECD TG 302B inherent biodegradability study (Zahn-Wellens test) on the Substance. The study is GLP compliant. The test material was ^{14}C-radiolabelled [redacted], reported to be uniformly labelled on both aromatic rings. The structure reported is for constituent 1. It is not indicated whether also other constituents were radiolabelled or only constituent 1. The test substance concentration was [redacted] µg/L. The study report states that modification of the standard test procedure was considered necessary because of the low water solubility of the test material (~ 70 µg/L). The inoculum was from a municipal wastewater treatment plant (inoculum concentration: mixed liquor suspended solids (MLSS) 1000 mg/L. The inoculum to test substance ratio was 19200 mg/mg. Total radioactivity in aquatic samples, organic extracts, and caustic traps, was determined. HPLC with radiochemical detection was used to study the distribution of the radiolabelled parent and transformation products. Mineralisation was 29% during 28 days. The decrease in ^{14}C-labelled test concentration was 91% in viable test and 8% in sterile control during 28 days. It was also reported that 12% of radioactivity was "*irreversibly sorbed or incorporated into biomass*" and based on the sum of this 12% fraction and the 29% mineralisation, you considered in the registration dossier that 41% was degraded. At the conclusion of the study, the mass balance for total radioactivity ranged from 78 to 88% for both the viable and killed control reaction mixtures. Most radioactivity remaining in the viable reaction mixtures consisted of water soluble ^{14}Cdegradation products which were not identified. You also stated in the dossier that the Substance is inherently biodegradable, using the criteria described in the OECD guideline. However, ECHA did not find the referred criterion in the OECD TG 302B test guideline.

- Section R.11.4.1.1.1 (page 42) of ECHA guidance R.11 (ECHA 2017b) includes two threshold values for the Zahn-Wellens test, i.e., 70% DOC removal for considering that the substance is not P and a lack of degradation (<20%) as evidence that the degradation in the environment would be slow. Therefore, a degradation of 41% would not be sufficient to exclude the P/vP concern. Moreover, due to the low test concentration and high inoculum to test material ratio, the conditions were more favourable to biodegradation than in a standard OECD TG 302B test and therefore ECHA considers that the study would not be suitable to exclude the P/vP concern, even in the (hypothetical) case where the threshold of 70% was reached. Correspondingly, even though the degradation in this case was above 20%, this does not exclude the possibility of slow degradation in the environment.

  Considering the high concentration of constituent 1, it can be concluded that constituent 1 was partly mineralised and underwent significant primary degradation into unidentified transformation products, which are potentially P/vP. For the other constituents, no conclusions can be drawn based on this study, due to their low concentrations.

  In your comments on the draft decision you agreed that the guideline (OECD TG 302B) itself contains no guidance on interpretation. You mentioned that the document titled 'Revised Introduction to the OECD Guidelines for Testing of Chemicals' (Section 3, Part 1, adopted 23 March 2006) states in Paragraph 36 that, *"Biodegradation above 20% of theoretical (measured as BOD, DOC removal or COD) may be regarded as evidence of inherent, primary biodegradability...".* Therefore your conclusion that the tested substance qualifies as inherently (primary) biodegradable relied on this reference. Regardless, you agreed that the result is "*inconclusive regarding reaching a definitive conclusion on persistence, according to REACh guidance on chemical safety assessment*".

- You have submitted a non-guideline inherent biodegradability study on the Substance. The study is GLP compliant. Non-labelled test substance was used. The structure of the test material ([redacted]) is indicated as the structure of constituent 1. It is not specified whether the analysis (GC-MS) was specific to constituent 1 or whether it relates to a sum of several constituents. Activated sludge from an industrial wastewater treatment plant was used as inoculum (inoculum concentration: MLSS ≥ 990 mg/L). Inoculum/test material ratio: 19800 mg/mg. The test material was present in the effluent treated by the sewage treatment plant where the inoculum was sampled. Thus, the inoculum was pre-exposed to the Substance. During seven days of incubation, background levels of [redacted] in the inoculum control mixtures decreased from 43.0 to 19.5 µg/L, a decrease of 55%. The concentration of [redacted] in test mixtures amended with 50 mg/L of the test material decreased from 94.0 to 24.7 µg/L, a decrease of 74%, during the same period. [redacted] concentrations in the sterile controls decreased 18%, from 95.2 to 78.5 µg/L, indicating that a major portion of the loss of the test material in the viable mixtures was due to biodegradation. The results indicate a significant primary degradation of constituent 1. For the other constituents, no conclusions can be drawn based on this study (it is not reported whether they were covered by the primary degradation measurements and even if they were, the concentration represents mainly the constituent 1 due to its high concentration). Due to the favourable conditions, i.e., the pre-exposure of the inoculum to the test substance and the high inoculum to test substance ratio, ECHA considers that these results cannot be used to rule out the potential persistence of the Substance.

- You have submitted an inherent biodegradability study using the Semi-Continuous Activated Sludge (SCAS) method, based on OECD TG 302A, on the Substance.

Degradation of 78% is reported. The measured parameter is not specified. However, according to the test guideline biodegradation is measured as the percentage elimination of organic carbon. No other information regarding this study is available. According to the OECD TG 302A, the method involves exposure of the test material to relatively high concentrations of micro-organisms over a long time period and the conditions are highly favourable to the selection and/or adaptation of micro-organisms capable of degrading the test material. Regarding inherent biodegradation test data, the ECHA guidance R.11 (ECHA, 2017b) states that only the results of a Zahn-Wellens test (OECD TG 302B) or MITI II test (OECD TG 302C) may be used to confirm that the substance does not fulfil the criteria for P provided that certain additional conditions are fulfilled. The guidance explicitly mentions that this possibility does not apply to the SCAS study. This means that the available SCAS study is not suitable to confirm that the Substance does not fulfil the criteria for P. The same guidance also states that lack of degradation (<20% degradation) in an inherent biodegradability test equivalent to the OECD TG 302 series may provide sufficient information to confirm that the P-criteria are fulfilled without the need for further simulation testing for the purpose of PBT/vPvB assessment. The results of the SCAS study do not fulfil this condition as you reported a degradation of 78%. ECHA considers that this result cannot be used to confirm the persistence or to rule out the potential persistence of the Substance or its constituents.

- In the REACH registration dossier for 1,2,3,4-tetrahydronaphthalene (i.e. tetralin; with EC number 204-340-2; constituent 6), as visible on ECHA's website, there is an OECD TG 301D closed bottle biodegradability test (OECD, 2004) with 5% degradation within 28 days and a BODIS test with 81% biodegradation (ECHA, 2021). The OECD study (2004) mentioned that "*Summarizing the available data on biodegradation, 1,2,3,4-tetrahydronaphthalene is not found readily biodegradable with every inoculum but is expected to be biodegraded well in the environment, though appropriate organisms may not be immediately available*". The BODIS test method is described as: "BODIS (Blok) Test (BOD-test for insoluble substances), Draft ISO Guideline 10708" and it is stated that "*The available BODIS test is regarded as key study and based on the above given arguments tetrahydronaphthalene can be considered as readily biodegradable. Moreover, there are numerous data that indicate that tetrahydronaphthalene is biodegraded by certain bacteria strains or that it is used as carbon and energy source.*" In this registration, the OECD TG 301D study is disregarded and it is explained that the difference in the biodegradability results was probably due to a much higher inocolum and test substance concentration used in the BODIS test compared to the Closed Bottle Test.

  ECHA notes that for the OECD TG 301 closed bottle test, the validity criteria are reported to be fulfilled and no deviations from the guideline are indicated. ECHA guidance R.11 (ECHA 2017b) refers to OECD TG 301 A-F and OECD TG 310 as ready biodegradation tests whereas the BODIS test is not mentioned. Appendix R.7.9—1 of ECHA guidance R.7b, (ECHA 2017c) contains a list of the ISO and OPPTS tests that are equivalent to the OECD guidelines listed above. The BODIS test or ISO 10708 are not included in that list. On the other hand, Richterich et al. (1998) mentions that the BODIS test (Two-Phase Closed Bottle test) is considered to have "entire compatibility" with the OECD tests for ready biodegradability (OECD TG 301) and to be particularly suitable for testing poorly soluble compounds. The design of the BODIS test method is mentioned to be completely congruous with the majority of the OECD 301 tests in terms of the test medium, strength of the inoculum, test duration etc. The respirometric test principle is comparable with the Closed Bottle test, i.e. the BOD is determined by measurement of dissolved oxygen in the test flasks (Richterich et al. 1998).

- In the registration for 1,2,3,4-tetrahydronaphthalene (EC number 204-340-2; constituent 6) there are also other screening studies available which have shown a low biodegradability (3% oxygen consumption in 20 days in a BOD study with synthetic seawater, 10% carbon dioxide production in 29 days in a mineralisation study with an adapted soil/sewage inoculum). A high degradation based on test material analysis was reported in a marine water study, but ECHA considers that the reliability of this result is questionable due to the high loss in evaporation control.

  For 1,2,3,4-tetrahydronaphthalene (constituent 6) non-guideline simulation tests have been published (Birch et al., 2017a, 2017b, 2018; Hammershøj et al., 2019; Prince et al., 2008). In these studies, several samples, considered to represent natural freshwaters, showed primary degradation half-lives ≤9.1 days and DT50s ≤18.2 days whereas two samples (taken from the same lake at different times, Birch et al. 2017b, 2018) showed higher half-lives (59.4 days and ≥56 days) and DT50s (62.4 days and ≥56 days), when converted to the reference temperature for freshwater (12°C). For marine water, one simulation test for constituent 6 is available and indicates a primary degradation half-life of 7.7 days, when converted to the reference temperature for marine water (9°C), whereas the DT50 is 14.4 days. However, all available simulation tests were conducted with hydrocarbon mixtures and therefore they are not suitable for supporting non-persistence even when the half-life is below the P criterion. In the studies by Birch et al. (2017a, 2017b, 2018) and Hammershøj et al. (2019), the quantification of degradation was based on the comparison of the concentrations in the viable tests and purified or deionised water controls and therefore the conditions of the viable tests and controls were not comparable e.g. in terms of the suspended solids, which may affect for example the formation of the non-extractable residues.

  Regarding the data for the marine water, the authors stated that the seawater samples were taken in the vicinity of a trafficked shipping port, which likely implied pre-exposure of the natural bacterial consortia to petroleum hydrocarbons (Birch et al., 2018).

Considering the available data and the fact that the BODIS study is not indicated as equivalent to OECD tests in the ECHA guidance (ECHA 2017c), ECHA considers that 1,2,3,4-tetrahydronaphthlane is potentially P or vP.

Evidence based on model predictions

ECHA considers that the BIOWIN and BioHCwin models (EPI Suite v4.11) are applicable for the constituents with some reservations. Their molecular weights are within the training set range.

For BIOWIN 1-4, the molecular fragments used for estimation do not cover the whole structures. The number of some fragments exceeds the maximum instances in the training set for BIOWIN 5–7 (all constituents) and for BioHCwin ((3-Phenylbutan-2-yl)benzene, i.e. constituent 4).

Based on the combination of the models BIOWIN 2 and 3 and the screening criteria in the ECHA guidance (ECHA 2017b), none of the constituents screens as potentially P or vP.

Based on the combination of models BIOWIN 3 and 6, all constituents screen as potentially P or vP. However, the value predicted by BIOWIN 3 is between 2.25 and 2.75 for all constituents, which means that more degradation relevant information is generally warranted (ECHA 2017b).

The BioHCwin model indicates a half-life of 57 days for constituent 4 thus indicating that

constituent 4 is potentially P or vP. For the other constituents the half-lives are 1-22 days but due to the inclusion of mixture studies in the training set of the model, ECHA considers that these results cannot be used to support non-persistence (ECHA, 2017b).

ECHA notes that the models used give the same results for constituents 1 and 2 ([redacted]) as these are positional isomers and they are recognized by these models as exactly the same set of molecular fragments. As these models are not developed to take into account this type of isomerism on biodegradability, the similarity of predictions for constituents 1 and 2 does not exclude potential differences in the biodegradability of constituents 1 and 2.

Conclusion on persistence

The available experimental data show that at least constituents 1 and 6 undergo primary biodegradation and mineralisation under certain conditions. As discussed above, the SCAS study (OECD TG 302A) is not relevant to confirm the persistence or to rule out the potential persistence of the Substance or its constituents. The other available studies on the Substance, i.e., the modified OECD TG 301B, the modified OECD TG 302B, and the non-guideline inherent biodegradation study, have used test conditions deviating from the standard ready or inherent biodegradation studies relevant for the cut-off values for screening tests in ECHA guidance R.11 (ECHA, 2017b) (i.e. for ready biodegradability, P/vP screening, or inherent degradability). Therefore, the results from these tests are not directly comparable to the cut-off values for screening tests. However, as the test conditions were more favourable to biodegradation than in standard ready or inherent biodegradability studies and the cut-off values were still not met, it can be concluded that constituent 1 is not readily biodegradable and not inherently biodegradable and that it is potentially P or vP. This conclusion is supported by the estimated data.

For the constituents 2, 3, 4, 5, and 6, the available experimental studies conducted on the Substance do not provide any information but due to the structural similarity between constituents 1 and 2, constituent 2 is considered also potentially persistent. For constituent 6, experimental data (screening tests and simulation tests) are available, indicating that constituent 6 is potentially P or vP.

No simulation test is available for the Substance or for the constituents, with the exception of 1,2,3,4-tetrahydronaphthalene (constituent 6). The test concentrations in the available biodegradation screening studies on the Substance were typical to OECD TG 309 surface water simulation studies and based on graphs with test concentration vs. time, in some of the studies degradation seemed to follow (pseudo) first-order kinetics and thus in principle the studies could allow estimation of first-order half-lifes. However, other test conditions (e.g. use of inoculum from a sewage treatment plant) were not in accordance with requirements for simulation tests to be used for deriving half-lives for persistence assessment so the studies cannot be used to estimate half-lives for comparison with the P/vP criteria.

Based on the available data the primary degradation of constituents 1 and 6 may be relatively fast in certain conditions although it is not known whether this would occur at standard test conditions. In addition, the prediction of degradation/ transformation products of constituents 1 and 2 by the eMSCA (Pathway Prediction System of the EAWAG Aquatic Research Biocatalysis/ Biodegradation Database[2] and QSAR profiling (EPI Suite v4.11) of predicted products (log Kow, BCF, biodegradability) (data not shown) indicates that there is a PBT/vPvB concern with some of the predicted primary degradation/ transformation products.

[2] http://eawag-bbd.ethz.ch/predict/

Based on the BIOWIN and BioHCwin results, all constituents are potentially P and potentially vP.

Therefore the available and current information is not sufficient to draw a conclusion on the potential hazard, and based on the available data, the concern for P/vP cannot be ruled out.

However, information on persistence is not requested in this decision as ECHA considers that information on the physico-chemical properties is needed first to clarify whether there is a B/vB concern with any of the constituents and this information will allow focussing any potential further testing on persistence on the most relevant constituent(s).

b) Potential B/vB properties of the Substance

If a substance fulfills the criteria in Section 1.1.2 or 1.2.2 of Annex XIII to REACH, it is considered to have bioaccumulative (B) or very bioaccumulative (vB) properties.

For the purpose of the B/vB assessment and to check whether the criteria are fulfilled, the information listed in Section 3.2.2 of Annex XIII must be considered, including bioconcentration factor (BCF) values. Notably, if the BCF value is >2000 or >5000, the Substance fulfils the criteria for B or vB, respectively.

First step of the B assessment is to compare the log Kow value of the Substance to the screening criteria. It is considered that substances with a log Kow value >4.5 have the potential to be taken up by the aquatic organisms due to hydrophobicity of the substance. For air-breathing organisms, non-biotransformed neutral organic substance with a log Koa ≥5 in combination with a log Kow ≥2 is considered to have a potential to biomagnify in terrestrial food chains and air-breathing marine wildlife as well as in humans, while the substances with log Kow <2 are being quickly eliminated by urinary excretion, and therefore do not biomagnify even though their log Koa is high.

Evidence based on experimental data

- An OECD TG 107 study is available in the registration dossier, which reports a log Kow value of 3.94 for the Substance. This would indicate that the screening criteria for B is not met. However, no information is available on the study to assess the reliability of this value.

- An experimental log kow value (OECD TG 107; Klimisch 2 assigned by the registrant) of 3.78 at 23℃ is available for 1,2,3,4-tetrahydronaphthalene (constituent 6) in the registration dossier of constituent 6. Detailed documentation of the study is not available. In addition, an experimental value of 3.49 is available in the EPISUITE v4.1 experimental database.

- Clement *et al.* (1980) investigated the accumulation of hydrocarbons (including alkylated tetralins) in bivalve mollusc *Macoma baltica* from seawater during a 180 day continuous exposure, followed by a 60 day depuration phase. The molluscs were exposed to a crude oil seawater dispersion at nominal concentrations of 0.03, 0.3 and 3 mg/L^{-1}. The eMSCA calculated BCF values for alkylated tetralins from the data presented in table 3 by Clement *et al. (1980)*. The calculated values varied between ca. 10200 and 23300. However, ECHA deems that these values cannot be considered reliable, as the seawater used for control and test organisms were contaminated with the test material. In addition, the test was conducted with a mixture. Nevertheless, in

the aqueous phase, the mean number of alkyl substitions (expressed as alkyl carbons per aromatic molecule) in tetralins was 3.4, while in the molluscs the mean substitution level was 4.8 (day 60) or higher increasing up to 5.7 by day 240. This would indicate that substituted tetralins (e.g., the main constituents) would have higher potential to bioaccumulate compared to the lesser substitued tetralins.

Evidence based on model predictions

- Log Kow values estimated with KOWWIN v1.68 for all constituents except 1,2,3,4-tetrahydronaphthalene (constituent 6) are above the screening criterion for bioaccumulation, ranging from 5.00 to 6.11. All constituents are within the molecular weight range and their structures are represented by the fragments in the model.

- Estimated log Koa values for all constituents are ≥ 5, which means that together with estimated log Kow they may fulfil the screening criteria for biomagnification in air-breathing organisms.

- BCF values for each constituent were estimated by the eMSCA using BCFBAF v3.01. Estimated regression-based BCF value of 5026 L/kg for the main constituents 1 and 2 indicates that they meet the criteria for vB. The models were not sensitive enough to differentiate between the two constituents, which are isomers differing only on the position of a functional group. Constituent 4 meets the criteria for B according to the estimated BCF-value of 2210.

- According to the Arnot-Gobas models, constituent 3 meets the criteria for B, if a parameter for biotransformation is included in the model. In the most conservative case, where biotransformation is assumed to not take place (i.e., it is set zero in the model), every constituent except constituent 6 meets the criteria for vB.

The available and current information is not sufficient to draw a conclusion on the potential hazard. Based on the estimated data, the concern for B/vB cannot be ruled out for the Substance. Therefore, further information is requested to clarify whether the constituents of the Substance meet the screening criteria for B/vB.

c) Potential T properties of the Substance

If a substance fulfils the criteria in Section 1.1.3 of Annex XIII to REACH, it is considered to fulfil the toxicity (T) criterion.

For the purpose of the assessment of T and to check whether the criteria are fulfilled, the information listed in Section 3.2.3 of Annex XIII must be considered, such as results of long-term toxicity tests. Also screening information of Section 3.1.2 to Annex XIII, such as short-term aquatic toxicity and QSAR predictions, should be considered in a weight-of-evidence approach to clarify the potential risk related to toxicity of the Substance.

Evidence based on experimental data

- You have submitted a long-term toxicity test on *Daphnia magna* (US EPA Section 797.1330) for the Substance. Significant effects on reproduction were observed for all tested concentrations resulting in a 21d NOEC value of <0.0019 mg/L for the Substance. Also another long-term toxicity test is available on *Daphnia magna* (OECD TG 211) for the Substance (Unpublished 2009b). The lowest 21d NOEC value of 0.0039 mg/L was observed for reproduction. The other observed toxicity values were a

21d NOEC value of 0.0277 mg/L based on parental survival and dry weight and a 21d NOEC value of 0.0142 mg/L based on parental length.

- You have also submitted a short-term toxicity test on *Daphnia magna* (unknown test method) with an EC50 value of 0.044 mg/L for the Substance. Another short-term toxicity test on *Daphnia magna* (OECD TG 202) is available with 48h EC50 value of 0.107 mg/L for the Substance (Unpublished 2009a).

- You have submitted a long-term toxicity test with fish (*Oncorhynchus mykiss*) according to draft OECD TG 215 resulting in a 28d NOEC value of 0.023 mg/L based on juvenile growth for the Substance. You have also submitted a short-term toxicity test according to OECD TG 203 with fish resulting in a 96h LC50 value of >0.038 mg/L for the Substance.

- You have also submitted one toxicity test for aquatic microalgae (*Pseudokirchineriella subcapitata*) according to OECD TG 201 (limit test at the limit of water solubility of the Substance). This study resulted a 72h NOEC value of <0.076 mg/L based on inhibition on algal growth for the Substance.

- ECHA notes that the Substance has not been classified according to CLP Regulation as carcinogenic, germ cell mutagenic, toxic for reproduction or specific target organ toxic after repeated exposure. There are no indications of the fulfilment of the T criterion in Annex XIII to REACH from the available mammalian toxicity data.

Evidence based on model predictions

The ECOSAR (v.1.11) QSAR estimations with estimated water solubility of 0.1688 mg/l (WSKowwin v1.43) and estimated log Kow of 6.114 for aquatic toxicity predict chronic toxicity values of 0.006 mg/L for fish, 0.009 for daphnid and 0.071 for green algae suggesting high chronic toxicity for the main constituents 6-(1-phenylethyl)-1,2,3,4-tetrahydronaphthalene and 5-(1-phenylethyl)-1,2,3,4-tetrahydronaphthalene.

The estimated acute toxicity values with same parameters are 96h LC50 0.039 mg/L for fish, 48h LC50 0.033 mg/L for daphnid and 96h EC50 0.177 mg/L for green algae.

The QSAR estimations indicate that the T criterion might be fulfilled for the main constituents 6-(1-phenylethyl)-1,2,3,4-tetrahydronaphthalene) and 5-(1-phenylethyl)-1,2,3,4-tetrahydronaphthalene based on long-term aquatic toxicity.

The available information for aquatic invertebrates suggests that the Substance may have T properties. The QSAR estimations suggest that the observed toxicity may be attributed to the main constituents of the Substance 6-(1-phenylethyl)-1,2,3,4-tetrahydronaphthalene and 5-(1-phenylethyl)-1,2,3,4-tetrahydronaphthale.

1.2 Potential exposure

According to the information you submitted in all registration dossiers, the aggregated tonnage of the Substance manufactured or imported in the EU is in the range of [redacted] per year.

Furthermore, you reported that the Substance is used as [redacted]. The Substance can be released to the environment as [redacted] from [redacted] using the Substance.

Therefore exposure to the environment cannot be excluded.

1.3 Identification of the potential risk to be clarified

Based on the weight of evidence from all information available in the registration dossier and information from the published literature, there is sufficient evidence to justify that the Substance may be a PBT/vPvB substance.

The information you provided on manufacture and uses demonstrates a potential for exposure of the environment.

Based on this hazard and exposure information the substance poses a potential risk to the environment.

As explained in Section 1.1 above, the available information is not sufficient to conclude on the potential hazard and in particular on the B property of the specific constituents of the Substance. Consequently, further data is needed to clarify the potential risk related to PBT/vPvB properties.

1.4 Further risk management measures

If the Substance is confirmed as meeting the P, B and T criteria or the vP and vB criteria it can be identified as a PBT or vPvB, respectively.

The evaluating MSCA will analyse the options to manage the risk(s). New regulatory risk management measures could be an identification as a substance of very high concern (SVHC) under Article 57 of REACH and a subsequent authorisation or a restriction of the Substance. This would result in stricter risk management measures than currently in place, such as minimisation of emissions, better waste management and revised instructions on safe use, if appropriate.

2. How to clarify the potential risk

2.1 Development of the testing strategy

The information resulting from the request will provide information on the potential B properties of the specified constituents of the Substance.

Following a "known constituents"-approach as indicated in section R.11.4.2.2.2 of ECHA guidance R.11. (ECHA 2017b), the known constituents of the Substance are then subjected to individual assessment. Later if necessary a reliable n-octanol/water partition coefficient (Kow) information may be needed for the consideration of further testing.

As a first step, n-octanol/water partition coefficient tests are requested where the specified constituents of the Substance have to be tested separately. This screening level information will constitute the first tier in a testing strategy to determine whether the screening criteria for B is met for the individual constituents of the Substance. The evaluating MSCA will review the information submitted as an outcome of the first tier of the testing strategy, evaluate whether further information is still needed to clarify the potential risk for PBT/vPvB properties and if necessary, select the relevant constituent(s) of the Substance for further testing of P/vP, B/vB and T properties. Further information may be needed in a follow-up decision making process in case one or more constituents will meet the screening criteria for B.

2.2 Partition Coefficient (1-Octanol/Water): Slow-Strirring Method (test method OECD TG 123) or HPLC method (test method: OECD TG 117)

a) Aim of the study

As explained in Section 1.1 above, information on the potential bioaccumulation properties of the Substance is not sufficient to draw a conclusion on the potential hazard.

A substance is identified as a PBT/vPvB substance if it includes at least one relevant constituent fulfilling the PBT/vPvB criteria. Constituents, impurities, and additives should normally be considered relevant for the PBT/vPvB assessment when they are present in concentration of ≥0.1 % (w/w) (ECHA 2017b).

The aim of the requested test is to obtain an n-octanol/water partition coefficient (Kow) values to determine whether the B screening criterion is met for the specified constituents of the Substance.

The partition coefficient n-octanol/water test is a standard information requirement at Annex VII of REACH (Section 7.8) and may be subject to a compliance check (Article 41 of REACH). As the Substance has been notified under the Directive 67/548/EEC, and you did not submit relevant new information in your registration dossier under REACH on top of information required under the Directive 67/548/EC, a compliance check under dossier evaluation for previously notified substance (NONS) is not applicable. The information requested in this decision aims at clarifying the potential risk that the Substance poses, in clarifying the Kow values of the specified constituents of the Substance.

An experimental log Kow value according to OECD TG 107 is available in the registration dossier with an unknown test material. ECHA assumes that this represents the partition coefficient n-octanol/water for the whole multi-constituent Substance and, therefore, cannot be used for the assessment of the bioaccumulation potential of the individual constituents. Furthermore the OECD TG 107 is not recommended for substances with a high expected log Kow (log Kow >4). Finally all estimated log Kow values for the constituents of the Substance present in the concentration of ≥0.1% (w/w) except 1,2,3,4-tetrahydronaphthalene (constituent 6) are above the screening criterion for bioaccumulation.

Thus, under the current substance evaluation, the partition coefficient n-octanol/water test according to OECD TG 123 or OECD TG 117 will not be performed on the Substance but instead on the specified individual constituents of the Substance.

b) Specification of the requested study

Test materials and their availability

The Substance is a multi-constituent substance with a known composition of constituents. You must test the following five constituents:

	Constituents	EC / List no.	CAS RN
1	[redacted]	-	[redacted]
2	[redacted]	-	[redacted]
3	[redacted]	-	[redacted]
4	[redacted]	-	[redacted]
5	[redacted]	[redacted]	[redacted]

To clarify whether the constituents of the Substance meet the screening criteria for B/vB, you must perform the test with each of the specified constituents of the Substance separately.

The constituents of the Substance specified in the request are commercially available. This request does not require any additional work on substance synthesis.

You commented that the initial CAS RN for ([redacted] (constituent 4, ie [redacted]) was specific to one possible diastereomer of that constituent, and that you intend to revise the CAS RN of this constituent using [redacted], which encompasses all isomers of this constituent. ECHA agrees that it is important to refer to that CAS RN encompassing all isomers of the constituent, and has amended the draft decision accordingly.

Choice of the test method

In your comments on the draft decision you requested ECHA to consider the OECD TG 117 (HPLC method) as an option to provide the requested information. You presented the following justifications for the requested change:

- Constituents 1 and 2 have a predicted log Pow value of 6.1, only modestly exceeding the recommended range in the HPLC method.
- The recommended reference substances in the HPLC method have a log Pow range of 0.3 to 6.5. You agreed with ECHA that the HPLC method may fail to yield accurate log Pow values if the reference substances are poorly selected.
- The individual constituents of the Substance are aromatic hydrocarbons chemically similar with each other and possess no functional groups associated with hydrogen bonding interactions, which may cause bias in the determination of log Pow in the HPLC method.
- For the screening purposes and the prioritization of the individual constituents of the Substance for further PBT testing, it should be possible to identify a set of simple aromatic hydrocarbon reference substances having well-established log Pow values.

ECHA notes that the Slow-stirring method (OECD TG 123) avoids the formation of microscopic octanol droplets in the water phase. In the HPLC method, the log Kow is not measured directly as it is in the OECD TG 123 but estimated from the correlation for a series of reference substances. Therefore the log Kow value depends on the quality of the other log Kow measurements (often measured by the Shake flask method) and the selection of reference substances (ECHA, 2017a). The uncertainties associated with extrapolations beyond the calibration range can be considerable (Tolls et al., 2003).

When considering the choice of methods, you should bear in mind that using the Slow-stirring method (OECD TG 123) to clarify the potential hazard allows direct determination of the log Kow of the specified potentially highly hydrophobic constituents of the Substance and does not depend on the selection of reference substances and, thus, could be more accurate. In case the HPLC method (OECD TG 117) is selected, the reference substances must be aromatic hydrocarbons having well-established log Kow values – in-line with your comments to the draft decision - and the highest log Kow value of the reference substance must be ≥6.5.

ECHA agrees however that for screening purposes and for the selection of the constituents for potential further persistency testing also, in principle, the OECD TG 117 can be used to obtain log Kow values. Thus, ECHA has amended the draft decision and you may choose

to perform either the OECD TG 123 or the OECD TG 117 for the determination of octanol/water partition coefficient.

Request for the full study report

You must submit the full study report which includes:
- a complete rationale of test design and
- interpretation of the results
- access to all information available, such as implemented method, raw data collected, interpretations and calculations, consideration of uncertainties, argumentation, etc.

This will enable the evaluating MSCA to fully and independently assess all the information provided, including the statistical analysis, and to efficiently clarify the potential hazard for the PBT/vPvB properties of the Substance.

c) Alternative approaches and how the request is appropriate to meet its objective

The request for the partition coefficient (n-octanol/water) test following either the OECD TG 117 or OECD TG 123 for specified constituents of the Substance is:

- Appropriate, because these tests are suitable and necessary to obtain information which will allow clarifying whether the individual constituents of the Substance fulfil the screening B criterion. This will enable the evaluating MSCA to decide, according to the "known constituent" approach, which is the most relevant constituent(s) for further testing, if necessary, to clarify the potential hazard.

- Testing on the specified constituents of the Substance is necessary to assess whether they meet the screening criterion for B. There is currently no experimental information available to assess if the B screening criterion is met for the other individual constituents of the Substance except 1,2,3,4-tetrahydronaphthalene (constituent 6). If more than one of the constituents fulfil the B screening criterion, the information on the partition coefficient n-octanol/water will provide a stronger basis for selecting the most relevant constituent(s) for further testing to clarify the potential risk for PBT properties. Currently, there is only predicted data available for comparing the B properties of the constituents.

- The least onerous measure, because there is no equally suitable alternative method available to obtain the information that would clarify the potential hazard. The other possible alternative is the Shake Flask Method (OECD TG 107). The applicability range of the HPLC method falls within the log Kow range 0 to 6 and the Shake flask method falls within the log Kow range -2 to 4. Thus, the Shake flask method would not be an appropriate test for highly hydrophobic substances. By contrast, the Slow-stirring method (OECD TG 123) can be used for very hydrophobic substances up to log Kow 8.3 (ECHA 2017a). In your comments on the draft decision you noted that the OECD TG 117 states that "*reverse phase HPLC method enables partition coefficients to be estimated in the log Pow range between 0 and 6 but can be expanded to cover the log Pow range between 6 and 10 in exceptional cases*".

  To select the relevant constituent(s) of the Substance for further testing and, thus to avoid unnecessary testing, ECHA considers that the request to perform a partition coefficient (n-octanol/water) test with either the OECD TG 117 or the OECD TG 123 with all the specified constituents of the Substance is the least onerous measure to clarify the potential risk.

d) Consideration of the time needed to perform the requested study

In your comments on the draft decision, you requested an extension of the deadline from 6 months to 9 months.

An extension of 6 months from the standard deadline has been exceptionally granted by ECHA to consider the current longer lead times in contract research organisations. ECHA notes that the selection of the test (OECD TG 117 or OECD TG 123) does not influence the delivery times of purchased constituents. However, this additional time is also sufficient to address the delivery times for the commercially available constituents having ≥95% purity.

Therefore, ECHA has modified the deadline of the decision and set the deadline to 12 months.

2.3 References relevant to the requests (which are not included in the registration dossier)

Birch H, Andersen HR, Comber M, and Mayer P (2017a). Biodegradation testing of chemicals with high Henry's constants separating mass and effective concentration reveals higher rate constants. *Chemosphere* 174, pp. 716-721

Birch H, Hammershøj R, Comber M, and Mayer P (2017b). Biodegradation of hydrocarbon mixtures in surface waters at environmentally relevant levels - Effect of inoculum origin on kinetics and sequence of degradation. *Chemosphere* 184, pp. 400−407.

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ECHA (2017c). Guidance on information requirements and chemical safety assessment, Chapter R.7b (version 4.0, July 2017).

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OECD (2004). SIDS 1,2,3,4-tetrahydronaphthalene. CAS N°: 119-64-2. UNEP Publications. (https://hpvchemicals.oecd.org/ui/handler.axd?id=9b99dd64-e50d-4f23-a6e5-c4135be56716 (accessed March 2022).

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319-326.

Study report (2009a). [redacted] RP Heat Transfer fluid: An acute toxicity study with the Daphnid, *Daphnia magna*. Unpublished study report.

Study report (2009b). [redacted] TM RP Heat Transfer Fluid: Chronic reproduction test with daphnids (*Daphnia magna)* under flow-through conditions. Unpublished study report.

Study report (2009c). Primary degradation in seawater study. Unpublished.

Tolls J. *et al.* (2003). Slow-stirring method for determining the n-octanol/water partition coefficient (Pow) for highly hydrophobic chemicals: performance evaluation in a ring test. *Environ Toxicol Chem.* 22(5), 1051-1057.

Appendix B: Procedure

This decision does not imply that the information you submitted in your registration dossier(s) are in compliance with the REACH requirements. ECHA may still initiate a compliance check on your dossiers.

12-month evaluation

Due to initial grounds of concern for PBT/vPvB and for exposure of environment, the Member State Committee agreed to include the Substance (EC No 400-370-7, CAS RN 63231-51-6) in the Community rolling action plan (CoRAP) to be evaluated in 2021. Finland is the competent authority ('the evaluating MSCA') appointed to carry out the evaluation.

In accordance with Article 45(4) of REACH, the evaluating MSCA carried out its evaluation based on the information in the registration dossier(s) you submitted on the Substance and on other relevant and available information.

The evaluating MSCA completed its evaluation considering that further information is required to clarify the following concerns: PBT/vPvB. Therefore, it submitted a draft decision (Article 46(1) of REACH) to ECHA on 16 March 2022.

Decision-making

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

For the purpose of this decision-making, dossier updates made after the date the draft of this decision was notified to you (Article 50(1) of REACH) will not be taken into account.

After the deadline set in this decision has passed, the evaluating MSCA will review the information you will have submitted and will evaluate whether further information is still needed to clarify the potential risk, according to Article 46(3) of REACH. Therefore, a subsequent evaluation of the Substance may still be initiated after the present substance evaluation is concluded.

(i) Registrant(s)' commenting phase

ECHA received your comments and forwarded them to the evaluating MSCA.

The evaluating MSCA took your comments into account (see Appendix A). The request(s) and the deadline (as explained in Section 2.2.d) were amended.

(ii) Proposals for amendment by other MSCAs and ECHA and referral to the Member State Committee

The evaluating MSCA notified the draft decision to the competent authorities of the other Member States and ECHA for proposal(s) for amendment.

As no amendments were proposed, ECHA took the decision according to Articles 52(2) and 51(3) of REACH.

After the deadline set in this decision has passed, the evaluating MSCA will review the information you will have submitted and will evaluate whether further information is still needed to clarify the potential risk, according to Article 46(3) of REACH. Therefore, a

subsequent evaluation of the Substance may still be initiated after the present substance evaluation is concluded.

Appendix C: Technical Guidance to follow when conducting new tests for REACH purposes

Test methods, GLP requirements and reporting

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.

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.

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].

Test material

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

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

   - 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*

   a) 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.
   b) The reported composition must include all constituents of each Test Material and their concentration values.

This information is needed to assess whether the Test Material is relevant for the Substance.

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

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