Helsinki, 17 December 2020

Addressees

Registrants of Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol listed in the last Appendix of this decision

Registered substance subject to this decision (the Substance)

Substance name: Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol
EC number: 264-848-5
CAS number: 64365-17-9

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. Ready biodegradability; test method: CO_2 in sealed vessels (Headspace test), OECD TG 310 (Request A.1), using the constituent 'Resin acids and Rosin acids, hydrogenated, monoesters with pentaerythritol' of the Substance, specified as follows:
    - the duration of the test must be extended to 60 days
    - the concentrations of the test substance must be analytically monitored during the test to determine primary degradation
    - if a conclusion that the monoester constituents of the Substance are not P/vP is drawn based on primary degradation, the identification of transformation/degradation products must be provided
    - two sterile controls must be included: 1) sterile controls as defined in the test guideline (i.e., with inoculated test medium) and 2) sterile controls with test medium but without inoculum
    - a toxicity control must be included

- you must report the carbon content of the test substance (weight percentage of carbon) and the molecular formulas of each of the components of the test substance.

Deadline

The information must be submitted by ***25 May 2022*** *from the date of the decision*

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 study 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 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] by Christel Schilliger-Musset, Director of Hazard Assessment

[1] As this is an electronic document, it is not physically signed. This communication has been approved according to ECHA's internal decision-approval process.

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 is necessary and appropriate.

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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

This decision follows the assessment of the available relevant information on the Substance ("HRPE"), which includes the degradation information provided by you for the monoester constituents of the Resin acids and Rosin acids, hydrogenated, esters with glycerol ("HRGE", EC number 266-042-9). This information was provided in response to the ECHA substance evaluation decision[2] requesting tiered PBT testing on the Substance. On this basis, the evaluating Member State and ECHA have concluded that the Substance may be a PBT/vPvB substance as defined in REACH Annex XIII.

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.

Assessment approach

According to ECHA Guidance R.11.4.1, a constituent should normally be considered relevant for the PBT/vPvB assessment when present in a concentration of ≥ 0.1% (w/w). The Substance is a UVCB containing, among other fractions, mono-, di-, tri-, and tetraesters of hydrogenated rosin acids with pentaerythritol; all of these fractions are

[2] SEV decision on EC 264-848-5 (7 February 2017)

present at concentrations of ≥0.1 % w/w. ECHA considers that the mono-, di-, tri-, and tetraester fractions are relevant for the purpose of the PBT/vPvB assessment.

Within each level of esterification, there is a high number of individual ester compounds, with different rosin acid moieties. There is a considerable structural similarity between the ester compounds within each level of esterification. Therefore, a "fraction profiling" approach is appropriate for the PBT/vPvB assessment of the Substance (ECHA 2017b: ECHA Guidance R.11.4.2.2.2).

In this context, constituents representing the different fractions of the Substance were profiled using QSAR models. The monoester fraction of the Substance was identified as the fraction with the highest potential for PBT/vPvB properties, on the basis of its higher bioaccumulation potential predicted by available QSARs. The di- tri-, and tetraesters are expected to have rather low bioaccumulation potential due to their physical and chemical properties (i.e., high molecular weights, large cross-sectional diameters of some components), slow uptake potential and low predicted BCF values (< 40). These constituents have predicted log Kow > 10, which indicates reduced bioavailability and bioaccumulation. Therefore, the P/vP assessment of the Substance is targeted on the monoester fraction.

Evidence based on experimental data

No simulation tests referred to in Annex XIII, Section 3.2.1(a), (b) or (c) are available for the Substance.

Regarding hydrolysis, no experimental data is available on the hydrolysis rate of the Substance or of its constituents. A non-guideline abiotic hydrolysis test on other esterified rosin substances (including, e.g., the substance Resin acids and Rosin acids, Esters with Pentaerythritol, CAS RN 8050-26-8) is available in your registration dossier. According to the study authors, this study proved the hydrolytic stability of the studied esters. The ester bonds are expected to be the main functional groups that would be susceptible to abiotic hydrolysis in these substances. ECHA notes that the Substance includes structurally similar ester constituents to the substances tested in this hydrolysis study (particularly, CAS RN 8050-26-8). Therefore, ECHA considers that the results of this study suggest that also the Substance and its constituents would be hydrolytically stable.

There are several ready biodegradability tests on the Substance available in your registration dossier. The observed degradation percentages range from 3 to 8.7%. The Substance is therefore not readily biodegradable and is considered to fulfil the screening criterion for persistence. It is noted that there is no information available on the degradability of individual constituents in the reported studies.

Evidence based on model predictions

Results from HYDROWIN QSAR models (HYDROWIN v2.00, U.S. Environmental Protection Agency, EPA 2010) show that it is unlikely that abiotic hydrolysis rates in environmentally relevant conditions would be sufficiently high to rule out the potential P/vP property for the monoester constituents of the Substance.

BIOWIN models were used to predict whether the screening criteria for P and vP (ECHA 2017b) are fulfilled for the monoesters of hydrogenated resin acids and rosin acids with pentaerythritol (referred hereafter as "pentaerythritol monoesters"). BIOWIN 1-4 models are not considered reliable for the selected constituents (THAA-mono-PE and DHAA-mono-PE[3]) as only a part of the molecular fragments is included in the applicability domain of these models. BIOWIN 5 and 6, which are applicable, give conflicting results, as discussed further below under "Assessment of the proposed read-across adaptation". Thus, no firm conclusion can be reached from the BIOWIN predictions and the fact that the Substance may have P/vP properties cannot be excluded on that basis.

Assessment of the proposed read-across adaptation

You have proposed in your registration dossier that the monoester fraction of HRPE does not need to be tested for ready biodegradability as you consider it possible to read across the results obtained in ready biodegradability studies according to OECD TG 310 conducted on the glycerol monoesters. ECHA notes that two OECD TG 310 studies have been conducted for the monoesters of hydrogenated resin acids and rosin acids with glycerol (referred hereafter as "glycerol monoesters") with test materials considered to be

[3] THAA-mono-PE: monoester of tetrahydroabietic acid with pentaerythritol; DHAA-mono-PE: monoester of dihydroabietic acid with pentaerythritol

representative of the monoester fraction of HRGE. These studies as a whole were considered acceptable to fulfil the information request made in a substance evaluation decision[4] for HRGE on ready biodegradability, allowing to conclude that the monoester fraction of HRGE is not P/vP.

ECHA has considered the scientific and regulatory validity of your read-across approach as further detailed below.

Annex XI, Section 1.5. specifies two conditions which must be fulfilled whenever a read-across approach is used. Firstly, there needs to be structural similarity between substances which results in a likelihood that they have similar physicochemical, toxicological and ecotoxicological properties so that the substances may be considered as a group or category. Secondly, it is required that the relevant properties of a substance within the group may be predicted from data for reference substance(s) within the group.

You have provided a read-across justification for the read-across between the monoester constituents of HRGE and of HRPE in Section 13.2 of your IUCLID dossier. In support of your adaptation you provided the following justification:

- *"[…] the only structural difference between glycerol and pentaerythritol mono-esters is the identity of the alcohol";*
- *"The QSAR predictions indicate that glycerol and pentaerythritol mono-esters have similar physicochemical properties. Pentaerythritol mono-esters have slightly higher molecular weights, and have slightly higher predicted Kow, Koc and BCF values […]"*
- *"When mono-ester constituents are degraded, the first step in the degradation process is likely to be breaking of the ester bond";*
- *"Glycerol mono-ester constituents contain two free hydroxyl groups, and pentaerythritol mono-ester constituents contain three" and "The additional functional group does not increase steric hindrance and thus would not limit the rate of degradation for these constituents […]This degradation process is expected to occur at a similar rate for both substances […]";*
- *"The degradation products from the expected primary degradation of both mono-ester fractions are resin acids and glycerol or […] pentaerythritol. The resin acids*

[4] SEv decision on EC 266-042-9 (7 February 2017)

would be the same for both mono-ester fractions. The other degradation product would be different but […] both glycerol and pentaerythritol are readily biodegradable"

- *"Based on these BIOWIN predictions, pentaerythritol mono-ester constituents may have more potential for biodegradation and therefore testing the glycerol monoester fraction and reading the results across to pentaerythritol mono-esters could be considered a worst-case approach."*

As explained above you intend to read across between the structurally similar substances, the glycerol monoesters as a source substance and monesters of HRPE as a target substance.

ECHA understands that you predict the properties of monoesters of HRPE using a read-across hypothesis which assumes that different compounds have the same type of biodegradation properties. The biodegradation properties of monoesters of HRPE are predicted based on a worst-case approach.

ECHA notes the following shortcomings with regards to prediction of biodegradation:

A) Annex XI, Section 1.5 of the REACH Regulation states that "*environmental fate* [properties] *may be predicted from data for reference substance(s)*". For this purpose "*it is important to provide supporting information to strengthen the rationale for the read-across*" (ECHA 2008: ECHA Guidance R.6.2.2.1.f). The set of supporting information should allow to verify the crucial aspects of the read-across hypothesis and establish that the biodegradation properties of the monoesters of HRPE can be predicted from the data on the glycerol monoesters.

Supporting information must include adequate experimental data to support that the rates of hydrolysis of the target and source substances are similar.

You indicate that the only structural difference between glycerol and pentaerythritol monoesters is the identity of the alcohol, i.e. glycerol and pentaerythritol, respectively. You claim that the first step in the degradation process is likely to be breaking of the ester bond and that the identity of the alcohol would not affect the hydrolysis rate. You explain that following hydrolysis, the target and source substances will release

similar resin acids. You explain that both glycerol and pentaerythritol are readily biodegradable and you conclude that the identity of the alcohol is not expected to affect the ultimate degradation potential of the monoester constituents of HRGE and HRPE.

ECHA notes that you have not provided any supporting information to demonstrate that the hydrolysis rate of monoesters of HRGE and HRPE are similar and that the identity of the alcohol has no impact on the prediction.

B) As indicated above, your read-across hypothesis is also based on the assumption that the studied glycerol monoesters constitute a worst-case for the prediction of biodegradation of the monoesters of HRPE. In this context, relevant, reliable and adequate information must be provided to support that the prediction of the properties of the target substance from the data on the source substance is conservative.

In support of your hypothesis you have provided the results of BIOWIN models 5 and 6 for representative structures of the monoesters of HRGE and HRPE (as these models are considered the most applicable to these structures) showing the following:

- mono-ester structures of HRGE are predicted 'readily biodegradable' based on BIOWIN 5 predictions but 'not readily biodegradable' based on BIOWIN 6;
- mono-ester structures of HRPE are predicted 'readily biodegradable' based on BIOWIN 5 predictions and some mono-ester constituents predicted 'readily biodegradable' based on BIOWIN 6 while others fail to reach the cut-off value (> 0.5) to be predicted to be 'readily biodegradable' (predictions range from 0.448 to 0.646).

You consider that the higher predicted biodegradation potential for pentaerythritol mono-ester constituents is likely to be due to the additional OH-group, leading to slightly higher water solubility and therefore higher biodegradation potential. Overall, you consider this information supportive of your worst-case hypothesis.

As explained above BIOWIN 5 and 6 give conflicting results in relation to the cut-off value for "readily biodegradable" and "not readily biodegradable" for some of the pentaerythritol monoester constituents. In addition, ECHA considers that there are

also other shortcomings in the BIOWIN models which weaken their relevance for the purpose of the read-across justification proposed by you. The differences in the BIOWIN 5 and 6 predictions between glycerol and pentaerythritol monoester of the same resin acid are based solely on the fragments in the alcohol moiety. ECHA considers that in this case the BIOWIN predictions are insufficient to estimate the potential impact of the structural differences on biodegradability and on the rate of hydrolysis of the ester bond. This is because BIOWIN models do not consider steric factors and assume additivity of fragments no matter what their type and number are (U.S. EPA 2012). Considering the alcohol moiety is close to the ester bond, the BIOWIN predictions do not rule out the potential higher steric hindrance of pentaerythritol moiety compared to the glycerol moiety. Such steric hindrance could be due to the extra hydroxyl group (despite the fact that it has a positive fragment coefficient in BIOWIN prediction, thus increasing the predicted probability of biogegradation), the larger molecular size (5 vs. 3 carbon atoms in alcohol moiety), or the higher degree of branching and the presence of a quaternary carbon in pentaerythritol mono-esters. These could potentially lead to a slower hydrolysis rate and therefore to potentially slower ultimate biodegradability rates of the pentaerythritol monoesters.

Due to the reasons above, ECHA concludes that the results of BIOWIN 5 and 6 provide insufficient support to conclude on the proposed worst-case hypothesis. Therefore, on the basis of the above, you have not provided adequate supporting information to support the claimed worst-case hypothesis.

In conclusion, you have not established that

- the monoesters of HRPE and HRGE are likely to have similar biodegradation properties due to similar hydrolysis rates
- the glycerol monoesters tested constitute a worst-case for the prediction of biodegradation properties of the monoesters of HRPE.

Therefore you have not provided sufficient supporting information to strengthen the rationale for the read-across.

As explained above, you have not established that the biodegradation of the monoesters of HRPE can be predicted from the data on the glycerol monoesters. Therefore, ECHA

considers that your adaptation does not comply with the general rules of adaptation as set out in Annex XI, Section 1.5. and that the validity of the read-across is not demonstrated.

You have provided additional considerations on the read-across. While these do not provide additional support to your adaptation, ECHA has addressed these considerations below:

You consider that the "*ability to produce a sample of the glycerol mono-ester with a higher proportion of mono-ester constituents* [compared to pentaerythritol mono-ester]" further support the read-across. However, while the ability to produce a sample with a sufficient proportion of monoesters is a prerequisite for testing , it is not a valid argument to justify the acceptance of your read-across adaptation. In addition, you have indicated that it is possible to produce a sample with 62% concentration of monoesters with pentaerythritol. ECHA considers that this is a sufficient concentration to conduct the requested study, provided that primary degradation is followed.

Finally, ECHA notes that OECD SIDS documents are available indicating that glycerol is readily biodegradable whereas pentaerythritol is not (OECD 2002 and 2005). In your comments you disagreed with the conclusion that pentaerythritol is not readily biodegradable since, according to the registered substance fact sheet, pentaerythritol is considered readily biodegrdable (ECHA 2020: Pentaerythritol factsheet). Furthermore, you note that this does not allow a conclusion that pentaerythritol monoesters will degrade slower than glycerol monoesters. ECHA agrees that the results from ready biodegradation studies on glycerol or pentaerythritol are not easily comparable to infer relative rates of degradation and notes that it has not concluded that pentaerythritol monoesters will degrade slower than glycerol monoesters based on the available information. Such a conclusion is not possible as there are currently no experimental data on the degradability of the pentaerythritol monoesters.

ECHA notes that the OECD TG 301C study (13.2% degradation based on test substance measurement after 28d) that is used in the OECD SIDS, is not included in the REACH registration for pentaerythritol. ECHA considers that the OECD SIDS documents suggest that pentaerythritol may be less biodegradable than glycerol. However, ECHA considers that for the current decision it is not necessary to draw any definitive conclusion on ready biodegradability of pentaerythritol or to assess further the potential reasons for the

different conclusions in the OECD SIDS document and by REACH registrant(s). ECHA also notes that theoretical maximum inorganic carbon production (ThIC) of the monoesters is mostly from the rosin moiety but the proportion of the alcohol moiety of the ThIC is somewhat higher for the pentaerythritol monoester. For example, for the glycerol monoester of dehydroabietic acid, the alcohol moiety contributes 13% of the ThIC whereas for the corresponding pentaerythritol monoester, the alcohol moiety contributes 20% of the ThIC (based on the carbon content of the alcohol and the monoester). Therefore, ECHA considers that the potential differences between degradability of glycerol and pentaerythritol cannot be excluded and these could affect also the ultimate degradation of the monoesters. There is no PBT/vPvB concern with these alcohols. However, these results mean that the CO_2 production of pentaerythritol monoesters in a ready biodegradation test could potentially be slower than of glycerol monoesters. This is not in accordance with your assumption that the glycerol monoesters constitute a worst-case for the prediction of biodegradation properties of the pentaerythritol monoesters.

In your comments you considered that the degradation pathways are similar between the glycerol and pentaerythritol monoesters. ECHA notes that for a conclusion "not P/vP" it is the rate of transformation (to non-PBT/vPvB products) which matters the most. A similarity of transformation pathway does not prove that also the rate of transformation would be similar. In addition, although the ester hydrolysis of a parent monoester would produce a rosin acid and an alcohol, the structure of the alcohol moieties differ between glycerol and pentaerythritol monoesters and therefore also the predicted transformation products differ between the two types of monoesters. Other transformations could occur before the ester hydrolysis. Even if the potential transformation products which still include an ester bond are likely to eventually undergo ester hydrolysis, it cannot be ruled out that the initial transformations, e.g. in the alcohol moiety, could affect the hydrolysis rate.

To conclude, the available information suggest that the Substance may have P or vP properties.

The available and current information is not sufficient to draw a conclusion on the hazard. Further information is needed on the P/vP properties of the constituent 'Resin acids and Rosin acids, hydrogenated, monoesters with pentaerythritol' as further described in Section 2 below.

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b) Potential B/vB properties of the Substance

If a substance fulfils 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. If no such data are available, it is necessary to consider the screening information of Section 3.1.2 to Annex XIII.

Section 3.1.2 of Annex XIII indicates that the indicator for the screening of bioaccumulation potential is the Log Kow determined experimentally or estimated by (Q)SAR models, provided they fulfil the criteria of Annex XI, Section 1.3. The threshold value for bioaccumulation potential provided in Section R.11.4.1.2.10 of REACH Guidance R.11 is a Log Kow value higher than 4.5.

There are no experimental bioaccumulation studies available on the Substance or its monoester constituent. The other information available on bioaccumulation properties of the Substance is described below.

Evidence based on experimental data

- The experimental log Kow results obtained by using the high-performance liquid chromatography (HPLC) method range from 4.6 - 7.3. However, no information on the individual constituents is available as the analytical peaks have not been identified.

Evidence based on model prediction

- The log Kow values predicted by KOWWIN model for selected individual structures are 5.78 and 5.70 for monoesterified pentaerythritol constituents, THAA-mono-PE and DHAA-mono-PE, respectively[3]. For the structures with a higher degree of esterification (di-, tri, and tetraesters of pentaerythritol constituents), the log Kow

values range from 12.16 to 27.71. The predicted Log Kow values are higher than 4.5 which indicates that these structures are potentially bioaccumulative.

- The QSAR predictions for BCFs using regression based model or Arnot-Gobas model for upper trophic levels (5% or 10.7% lipid content with zero biotransformation) range between 3038-19300 and 2669-18340 L/kg for THAA-mono-PE and DHAA-mono-PE constituents, respectively. For di-, tri- and tetraesters of pentaerythritol, the predictions show very low BCF values.

The available information suggests that the Substance may have B or vB properties.

The available and current information is not sufficient to draw a conclusion on the hazard.

Further information on the B/vB properties might be requested in a follow-up decision making process if needed to clarify the potential risk related to the PBT/vPvB properties.

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 3.1.3 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

- No long-term aquatic toxicity tests are available for the Substance or its monoester constituents.
- You have submitted short-term aquatic toxicity tests with fish (OECD TG 203), Daphnia (OECD TG 202) and algae (OECD TG 201), which applied water accommodated fractions (WAF) of several UVCB rosin substances belonging to the same rosin substance category. Aquatic short-term toxicity tests showed no toxic effects within the nominal test concentrations with loading rates up to 100 or 1000 mg/L with the exception of one Daphnia test, EC50 27 mg/L for a structural analogue Resin and rosin acids, hydrogenated, esters with methyl. The results are considered to be unreliable for PBT assessment of the Substance because the actual composition and concentration of the test material are not known and the concentrations decreased significantly during the tests.

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. Further information on these endpoints is expected under dossier evaluation .

Evidence based on model predictions

ECOSAR (v1.11) QSAR predictions offer very limited possibilities for predicting the ecotoxicity of the Substance as the applicability is restricted by low water solubility and high lipophilicity of the constituents. Only monoesterified pentaerythritol constituents fit the ECOSAR model (class esters), with chronic toxicity values (ChV) (algae) 0.099 mg/L, ChV (Daphnid) 0.112 mg/L and ChV (fish) 0.012 mg/L for THAA-mono-PE, and ChV (algae) 0.110, ChV (Daphnid) 0.129 mg/L and ChV (fish) 0.014 mg/L for DHAA-mono-PE. The lowest ChV values for fish (0.012 and 0.014 mg/L) are close to the T criterion for long-term aquatic toxicity (NOEC < 0.01 mg/L).

Only monoesters of the known constituents of the Substance are slightly water soluble (0.02 - 8.5 mg/l, according to modelling results with EPISuite/WSKOW and WatSol) and hence potentially more bioavailable than di-, tri-, and tetraesters, which are practically not water soluble. This is also seen with other rosin ester analogues: only monoesters are

slightly water soluble according to modelling results. Therefore, it can be estimated that monoesterified rosin ester structures are potentially the most toxic rosin ester constituents.

The available and current information is not sufficient to draw a conclusion on the potential hazard. Further information on the T property might be requested in a follow-up decision making process if needed to clarify the potential risk related to the PBT/vPvB properties.

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 100 – 1000 tonnes per year.

Furthermore, you reported that among other uses, the Substance is used:

- eg. in closed or batch processes, production of preparations by tabletting, compression, extrusion and pelletisation in formulation;
- eg. as processing aid, monomers for manufacture of thermoplastics, in coatings, cleaning agents, binders, release agents, adhesives, in rubber production and processing by industrial workers;
- eg. in roller application and spraying, treatment of articles, as laboratory reagent, cleaning agents, adhesives, road and construction applications and agrochemicals by professional workers;
- eg. in coatings, adhesives, sealants, anti-freeze and deicing products, biocidal products, paints, thinners, plasters, modelling clay, surface treatment products, inks, leather tanning, dye, impregnation, lubricants, greases, polishes, wax blends, cleaning products, fragnances, cosmetics and agrochemicals by consumers;
- in articles containing adhesives and sealants.

The Substance can be released to the environment as emissions from manufacturing plants, emissions from industrial and professional facilities using the Substance, consumer uses and uses from articles leading to emission to municipal waster water treatment plants.

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 hazard and in particular on the P/vP property. Consequently further information is needed to clarify the potential risk related to PBT/vPvB properties.

1.4 Further risk management measures

Currently there is no harmonised classification on the Substance, thus no obligatory hazard or precautionary statements are required. If the Substance is confirmed as meeting the P, B and T or vP and vB criteria in this and potential follow-up decision making process, it can be identified as a PBT/vPvB. The evaluating MSCA will analyse the options to manage the risk(s) and will assess the need for:

- further regulatory risk management in the form of identification as a substance of very high concern (SVHC) under Article 57 of REACH;
- 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

As a first step, a ready biodegradation test on the monoester constituents of the Substance is needed. The eMSCA will assess the information submitted by you, together with other available data, and will decide whether further information is needed to clarify the P/vP, B/vB, or T properties. The ready biodegradation test may allow to conclude that the monoester constituents of the Substance are not P/vP whereas it may not allow a definitive conclusion that they are P or vP. If a conclusion "not P/vP" cannot be drawn for the monoester constituents, further testing (e.g. a simulation test) may therefore be needed to clarify the P/vP property. If the eMSCA considers that further information is needed it will submit a new draft decision.

2.2 Request A.1 (Ready biodegradability; test method: CO_2 in sealed vessels (Headspace test), OECD TG 310) on the monoester constituents of the Substance

a) Aim of the study

The aim of the test requested is to conclude whether the Substance screens as P/vP and whether further testing is necessary to clarify the potential risk related to the PBT/vPvB properties.

In general, a ready biodegradation study provides information which can be used for concluding that a substance is not P/vP, or that it is potentially P/vP. However, for a definitive conclusion that a substance is P or vP, a degradation half-life obtained from a simulation test is generally needed. In the present decision a ready biodegradation test is requested as a first step for the P/vP assessment, based on the following considerations:

- The primary degradation of the glycerol monoesters in the ready biodegradation tests was relatively fast, probably due to fast hydrolysis of the ester bond; thus there is the potential that the primary degradation of the monoester constituents of HRPE in a ready biodegradation test will be fast which could, together with other available data, allow to conclude that the monoester constituents of the Substance are not P/vP.

- The production of radiolabelled constituent 'Resin acids and Rosin acids, hydrogenated, monoesters with pentaerythritol' may not be technically possible and results from a simulation test with no radiolabelling would be more difficult to interpret (as limited information would be available e.g. on mineralisation and on formation of non-extractable residues (NER)).

- The available ready biodegradability tests on the glycerol monoesters have been considered when specifying the test design of the new study on the pentaerythritol monoesters in the decision (for example, the requirement for two different types of sterile controls is based on the experience from the OECD TG 310 studies on the glycerol monoesters); with the specific modifications to the standard test protocol, ECHA considers that the likelihood to obtain valid results is high.

If the ready biodegradation test result will not enable concluding that the monoester constituents of the Substance are not P/vP, the eMSCA will consider the need for further testing (e.g., a degradation simulation test) to clarify the PBT/vPvB properties. If it is demonstrated that the monoesters undergo sufficient degradation (i.e. in OECD TG 310 ≥60% of the ThIC of the monoesters) in 28 days then it can be concluded that the monoesters are not P/vP. If the inorganic carbon (IC) production of the monoesters does not reach ≥60% of ThIC of the monoesters in 28 days, then all available results (including the extended test period) should be considered for the conclusion.

A ready biodegradability test (e.g. OECD TG 310) is a standard information requirement at Annex VII, Section 9.2.1.1 of REACH. It could therefore be subject to a compliance check under Article 41 of REACH. However, the current study request is to clarify the degradability of specific constituents of the Substance and will therefore not be performed on the registered Substance but instead on a test substance representative of the monoester constituents of the Substance. Also, several additions to the standard test guideline are required, such as analytical monitoring of the test material, monitoring of primary degradation and transformation/degradation products. Since non-standard parameters are required and the information request is based on a potential risk that the Substance poses, the request is necessary under the current substance evaluation.

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b) Specification of the requested study

Test material and concentration

The sample of the substance to be tested must represent the monoesterified pentaerythritol constituents of HRPE. This is because the monoester fraction of the Substance was identified as the fraction with the highest potential for PBT/vPvB properties, on the basis of its apparent bioaccumulation potential indicated by the QSAR analyses.

The sample to be tested can be a fraction of the Substance (UVCB), or a specifically manufactured substance, consisting of monoesterified pentaerythritol constituents as far as technically possible. In your read-across justification report you have indicated that it has been possible to produce a sample containing 62% of pentaerythritol monoester. ECHA considers that this concentration of the monoesters would be sufficient.

It is the responsibility of all the Registrant(s) to agree on the test material and to document the necessary information on composition of the test material. The substance identity information of the Substance and of the sample tested must enable the evaluating MSCA and ECHA to confirm the relevance of the testing for the Substance subject to substance evaluation.

When performing, documenting and interpreting the test you need to consider the likely situation that the test substance does not consist solely of the monoester constituents but it may contain constituents (e.g., rosin acids, pentaerythritol), which can be also produced in the degradation of the monoesters.

Degradability and carbon content may vary between the different constituents of the test substance and therefore the different constituents of the test substance may have degraded to a varying extent over the duration of the test. Therefore, for the assessment of the degradability of the monoester, you must report the carbon content of the test substance (weight percentage of carbon) and general molecular formulas for each of the components of the test substance (such as rosin acids and tetra-, tri-, di-, and monoesters of pentaerythritol)[5].

[5]The general molecular formulas are needed in particular to determine the carbon content of the constituents. The general molecular formulas can be estimated based on information available to the Registrant(s), e.g., on the composition of source substances which are used for the synthesis of the test substance. For example, molecular formulas of the mono-, di-, and triesters in which rosin

In your comments you noted that it takes a significant amount of time to produce enough yield of the test substance for all of the work proposed. According to you, this involves multiple purification steps in which the yield of monoester is reduced at every stage of the purification process. You proposed to produce one batch of test substance to be used for all of the proposed analysis and testing to avoid any potential issues with test substance identity and composition. ECHA agrees that it is important to produce one batch of test substance that is sufficient for the requested study.

Analysis of the test material and determination of primary degradation of the monoesters

It may be possible to conclude "not P/vP" based on primary degradation. Thus, in case it cannot be demonstrated that ≥60% of the ThIC production of the monoesters has been achieved, the extent of primary degradation of the monosters can be used to evaluate whether the Substance does not screen as P/vP as the final hydrolysis products of the monoesters are not PBT/vPvB.

The amount of the monoesters remaining in the test bottles must be analytically determined and quantified in relation to the initial amount, to verify whether degradation of the monoester constituents is occurring, and to determine the primary degradation of the monoesters. The frequency of the monoester measurements must follow the guidance given in OECD TG 310 (paragraph 49). It is important that the results allow the comparison between the degradation curves based on primary degradation and ultimate degradation.

The concentrations of the di-, tri- and tetraesters must be determined at least at the beginning of the study (zero time), after 28 days, and at the end of the study. The reason for the measurement of the di-, tri- and tetraesters is that these constituents may degrade to monoesters and to CO_2 during the study. With the measurements of these constituents, the contribution of these constituents to the monoester concentrations and CO_2 production can be estimated, which is important for the calculation of the primary and ultimate degradation of the monoesters.

acid moieties consist of the most common rosin acid in the source substance can be used, if the carbon content is considered to be representative for the constituent fraction. According to Environment Canada (2011, page 3) the most common rosin acids have the molecular formula C_{20} H_{30} O_2. This formula can be used if appropriate for the test substance. Experimental determination of molecular formulas of the different constituents of the test substance is therefore not necessarily needed.

The analyses should be done so that, for each of the measured constituents, both the amount in the test medium and the amount in the solvent rinse are taken into account (either by analysis of combined fractions, or separate analyses of both fractions). It was observed in the OECD TG 310 study on the glycerol monoesters that most of the monoesters were detected in the solvent rinse of the bottles.

The analytical techniques used must have sufficient sensitivity to analyse and quantitate the constituents of the test substance for the purposes of the test.

ECHA notes that measurements of the concentrations of di-, tri- and tetraesters are not necessarily needed in the following situation:

- The primary degradation of the monoesters is so low that a "not P/vP" conclusion from the current study can be ruled out even without measuring the concentrations of the higher esters. ECHA considers that this condition applies when it can be demonstrated that, during the whole study, $m_t/m_0 \geq y$ is fulfilled, where

  m_t = *amount of the monoesters in the test system at a given time point during the study (mg/L)*

  m_0 = *initial amount of the monoesters in the test system (mg/L)*

  $y = [(0.6 \times m_{initial}) + (m_{produced\_max})]/(m_{initial})$

  Details for this calculation are given in the footnote[6]. The rationale for using this calculation is that if the primary degradation of the monoesters, based

[6] $m_{initial}$ =initial concentration of the monoesters in test substance (mg/L); $m_{produced\_max}$=maximum theoretical increase in the concentration of monoesters (mg/L) from the hydrolysis of the di-, tri-, and tetraesters present in the test substance based on the concentrations of these esters in the test substance and on the consideration that for each molecule of the higher esters, one molecule of monoester can be produced; the calculation can be performed based on the molecular weights of the most common ester constituents (for example, esters of dehydroabietic acid can be used as the basis for the calculation, if considered representative for the test substance)); as an example, if the test system includes 10 mg/L of test substance with concentrations of mono- and di-, tri- and tetraesters of 62%, 29%, 0%, and 0%, respectively there are 6.2 mg/L of monoesters and 2.9 mg/L of diesters present and therefore, $m_{produced\_max}$ =*[(2.9 mg/L) x (422.61/709.10)] = 1.728 mg/L* any

on this simplified calculation, is less than 40%, then degradation in the conditions of the current test system is so low that a "not P/vP" conclusion for the monoesters would not be possible even if the calculation was refined based on the measured concentrations of the di-, tri-, and tetraesters. The <40% degradation is chosen based on the consideration that the ultimate degradation pass level based on % of ThIC for "not P/vP" is 60% (even if at a given % ThIC, the percentage of primary degradation is expected to be higher), and further 20% was subtracted due to the potential increased uncertainty of the primary degradation determination compared to ultimate degradation measurement. ECHA notes that if the $m_t/m_0 \geq y$ condition is not fulfilled, this still would not indicate that the monoesters are not P/vP but it would indicate that a more detailed analysis of the results (including, e.g., measured concentrations of the di-, tri-, and tetraesters) is needed.

As it is not possible to know beforehand whether the above-mentioned situation will be realised, you can consider storing samples during the study and postponing the decision on whether to analyse di-, tri- and tetraesters until the study has been completed and the results for CO_2 and for the monoesters are known (within the timeline set in this decision). However, for such an approach it must be demonstrated that the storage of the samples does not affect the reliability of the measurements.

Test duration

The duration of the test must be extended to 60 days. This is necessary because it is possible that a complete degradation of the monoesters is not achieved during 28 days and in that case it is important to monitor whether the degradation of the monoesters stops or whether it continues still after 28 days. ECHA notes that in the OECD TG 310 studies on the glycerol monoesters, the degradation of monoesters of ≥60 %ThIC during 28 days was not achieved and also the primary degradation of the monoesters during the study was not complete. However, the results (including extended test period) indicated a consistent decrease, which, together with other available data, allowed to conclude that the glycerol monoesters are not P/vP.

= 0.879 (422.61 and 709.10 are the molecular weights of mono- and diester of dehydroabietic acid with pentaerythritol)

According to the guidance (ECHA 2017b), degradation during the extended study period can in certain cases be used as evidence that the substance is not P/vP, together with other supporting information. The preconditions in the guidance (ECHA 2017a, 2017b) for using an extended test period for concluding "not P/vP" are based on the study results. E.g., the degradation curve should show that biodegradation has started but that the plateau has not been reached by day 28, and ≥60 %ThIC should be used as the criterion for concluding "not P/vP". The suitability of the extended study period for concluding "not P/vP" can therefore be assessed only when the study results are available. In case that the results do not fulfil the guidance preconditions for concluding "not P/vP" based on ultimate degradation, the results of the extended study period will still be used as a part of a weight-of-evidence approach (including primary degradation).

You may also consider other techniques to determine the biodegradability of poorly water-soluble chemicals in accordance with ECHA guidance (ECHA 2017a).

Sterile controls

Sterile controls as defined in the OECD TG 310 (i.e., including inoculated test medium) and sterile controls with test medium but without inoculum must be included to verify the contribution of abiotic phenomena including adsorption processes and hydrolysis to any observed removal of the test substance.

For the sterile controls, you should select the most suitable toxicant/sterilising agent and the appropriate conditions (such as the concentration of the toxicant), and give a justification.

The reason for the requirement of sterile controls with test medium but without inoculum is to determine whether the extractability of the test material changes during the study (in the absence of inoculum) and whether abiotic hydrolysis occurs under the conditions of the test. In the OECD TG 310 study with glycerol monoesters, there was a significant decrease of the monoesters also in the sterile controls and it remains unclear whether this was e.g. due to hydrolytic enzymes present in the inoculum (which may have been still

active), or whether this was due to the possible effects of the toxicant[7] on the extractability or analysis of the monoesters. In addition, CO_2 production in the study may be lower than in the studies performed on the glycerol monoesters, due to the potentially lower degradability of pentaerythritol compared to glycerol, a lower concentration of the monoesters compared to the test substances used for the glycerol monoesters, and the likely presence of di-, tri, and tetraesters in the test substance. Therefore, it may be more challenging to quantify to what extent the decrease in the monoester concentration is due to biodegradation. The inclusion of two different sterile controls is expected to help in this quantification.

The methods for the extraction and analysis of the monoesters must be validated also under the conditions of the sterile controls, in addition to the validation for the conditions of the active test. Thus, for example, if a toxicant is used in the sterile controls, the validation must be done in the presence of the toxicant at the concentration used in the study. ECHA notes that the analytical method for the glycerol monoesters was not validated with the toxicant (formaldehyde) and the recovery percentages of the monoesters (% of applied amount) in the beginning of the study were lower in the sterile controls than in the active tests, suggesting a possible effect of formaldehyde.

Identification of transformation/degradation products

In case it cannot be demonstrated that ≥60% of the ThIC production of the monoesters has been achieved, primary degradation can potentially be used to conclude that the monoesters are "not P/vP". In that case, the identification of transformation/degradation products of the monoesters is required for the assessment of PBT/vPvB properties. In the present case, there is predicted information that pentaerythritol (or oxidised derivatives of the pentaerythritol moiety) and resin acids are likely transformation products of the pentaerythritol monoesters. In case there are indications of transformation/degradation products of the monoesters which could contribute to the PBT/vPvB properties, these should be identified and quantified (i.e. whether the degradation of the monoesters leads to transformation products with PBT/vPvB properties). The importance of transformation products for the conclusion is particularly high if CO_2 production from the monoesters does not reach ≥60 % of ThIC of the monoesters, or if it cannot be accurately quantified. To

[7] Formaldehyde was used, at a concentration of 18 500 mg/L, which is significantly higher than indicated in OECD TG 301 or OECD TG 309.

quantify the amount of the relevant transformation products produced during the test, in particular the known hydrolysis products of rosin esters, their initial concentrations in the test substance need to be known.

In your comments you noted that the concentrations of degradation products may be too low to quantify adequately. ECHA considers that identification and quantification of transformation products is usually needed whenever mineralisation is not sufficient to rule out PBT/vPvB concern. Therefore, the same need would likely also apply to the alternative options to clarify the P/vP property, i.e., simulation tests. ECHA notes that in a simulation test there would be likely more challenges in the quantification of the transformation products due to the lower test substance concentration. ECHA considers that the lack of test substance consisting solely of the monoesters is not an acceptable reason for not requesting the study or for not identifying and quantifying the transformation products. Assuming a test substance with a 62% monoester concentration, the concentrations of the transformation products can be expected to be ca. 0.6-fold compared to a test substance consisting solely of the monoesters. ECHA does not regard this as a significant difference for the sensitivity of analytical methods. In addition, ECHA notes that you have not provided any specific justifications why the quantification of degradation products would be a problem in the present case. ECHA considers that it is an advantage of screening tests compared to simulation tests that a higher test concentration can be used. ECHA understands that the same transformation products (such as resin acids) can be produced also from other constituents than monoesters, which complicates the interpretation of the results. However, with simultaneous measurements of the other constituents, their contribution to the transformation products can be estimated. It is important to determine the relevant transformation products for the reasons stated above, to the extent technically possible (see also Appendix C). You should report the potential problems encountered in quantifying or identifying the transformation products.

ECHA notes that identification and quantification of transformation products is not necessarily needed in the following two situations:

- The ultimate degradation (supported by primary degradation measurement) allow concluding that the monoester constituents of the Substance are not P/vP. ECHA notes that the measurement of transformation products should

be omitted on this basis only if discussed and agreed with the evaluating MSCA based on the results for CO_2 and for the mono-, di-, tri-, and tetraesters, both in the active tests and in the sterile controls. This is because the ultimate and primary degradation of the monoesters need to be assessed by taking into account all these results. It is not possible to define in the current decision all potential result scenarios and their interpretation, due to the expected complexity and yet unknown composition of the test substance to be used.

- The primary degradation of the monoesters is so low that a "not P/vP" conclusion from the current study can be ruled out even without consideration of transformation products. ECHA considers that this can be demonstrated by the condition that, during the whole study, $m_t/m_0 \geq y$ is fulfilled. The equation $m_t/m_0 \geq y$ is explained above under '*Analysis of the test material and determination of primary degradation of the monoesters'*. ECHA considers that if $m_t/m_0 \geq y$ is fulfilled during the whole study, then a "not P/vP" conclusion for the monoesters is ruled out and, consequently, information on transformation products is not needed. ECHA notes that if the $m_t/m_0 \geq$ y condition is not fulfilled, this still would not indicate that the monoesters are not P/vP but it would indicate that a more detailed analysis of the results (including the measurements of transformation products), is needed.

As it is not possible to know beforehand whether one of the two above-mentioned situations will be realised, you can consider storing samples during the study and postponing the decision on whether to analyse the transformation products until the study has been completed and the results for the other parameters to be measured are known (within the timeline set in this decision). However, for such an approach it must be demonstrated that the storage of the samples does not affect the reliability of the measurements.

Toxicity control

A toxicity control must be included and if inhibition by the test substance is suspected the test can be repeated as instructed in the test guideline (OECD TG 310), using, e.g., a lower test substance concentration.

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 analytical data, and to efficiently clarify the potential hazard for the PBT/vPvB properties for the Substance.

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

The request is:

- Appropriate, because the test is suitable and necessary to obtain information which will allow clarifying whether the monoester constituents of the Substance fulfil the screening criterion for P/vP and thus whether further information would still be needed to clarify the P/vP property.
- The least onerous measure, since by conducting a ready biodegradability test, the need for simulation testing will be avoided in case a conclusion that the monoester constituents of the Substance are not P/vP can be drawn.

Of the different ready biodegradation test protocols (OECD TG 301A-F, OECD TG 310), the CO_2 in sealed vessels (Headspace test) (OECD TG 310), has been selected taking into consideration the information obtained from you during the substance evaluation process

and the experience obtained with the OECD TG 310 studies conducted for the glycerol monoesters. In addition, the OECD TG 310 test is based on CO_2 production. ECHA considers this as an advantage over tests on O_2 consumption or removal of dissolved organic carbon (DOC). CO_2-C is directly derived from the test substance whereas O_2 consumption is an indirect indication of biodegradation and the ratio of O_2 consumption to CO_2 production may vary between compounds. Thus, CO_2 measurements provide better possibilities for calculating the biodegradation of the monoesters, using the proportions of the different constituents of the the total carbon in the test substance. Such calculations were considered important in the assessment of the OECD TG 310 studies on the glycerol monoesters and they may be also important for the pentaerythritol monoesters as the CO_2 production of the test substance may be lower as explained above under "Sterile controls".

In your comments on the draft decision you conceded that there is no experimental data to suggest that the initial hydrolysis rates would be similar for HRGE and HRPE monoesters and further work on the pentaerythritol monoesters would therefore be required. Instead of conducting the requested OECD TG 310 study as the first measure, you proposed the following tiered testing approach:

Tier 1: Demonstrate that the ester hydrolysis of HRPE monoesters is not significantly different to the HRGE monoesters by conducting an experimental hydrolysis study in HRPE monoesters, conducted to OECD guidelines and GLP.

Tier 2: Conduct additional method development and feasibility studies as you considered that there are increased challenges conducting an OECD TG 310 study on the pentaerythritol monoesters in comparison with the glycerol monoesters. You proposed that a non-GLP feasibility study is undertaken to identify and overcome challenges with the conduct of the studies and the analysis. You noted that you would like to discuss the results and outcome of the feasibility study with ECHA before deciding if a full definitive Study would still be required or whether this would be feasible.

Tier 3: Perform the Definitive Study using the most suitable methodology identified in Tier 2 but only once the conduct has been agreed with ECHA if it is still feasible.

ECHA notes that you did not specify the test guideline for the hydrolysis study proposed as Tier 1. Therefore, ECHA understands that your proposal would be an abiotic hydrolysis study based on an OECD test guideline (OECD TG 111: Hydrolysis as a function of pH).
ECHA agrees with your reasoning that if the pentaerythritol monoesters undergo sufficient primary degradation (e.g., through hydrolysis) to transformation products which are not PBT/vPvB, then the pentaerythritol monoesters could be considered 'not P/vP'. However, ECHA considers that your proposed hydrolysis study would not clarify the P/vP property for the following reasons:

- There is no evidence that the glycerol or pentaerythritol monoesters of hydrogenated resin acids and rosin acids would undergo abiotic hydrolysis.
- The above-mentioned hydrolysis test on other esterified rosin substances did not indicate hydrolysis. Furthermore, the report provides no information on the deviation of the reported results, (e.g. replicate bottles or replicate analytical measurements), so the reliability of the reported monoester concentrations cannot be assessed.
- There are no standard hydrolysis studies available for the glycerol monoesters and no other information indicating abiotic hydrolysis of the glycerol monoesters. Therefore, it is not possible to demonstrate with an abiotic hydrolysis study on the pentaerythritol monoesters that the abiotic ester hydrolysis of pentaerythritol monoesters is not significantly different to the glycerol monoesters. Such a demonstration would require abiotic hydrolysis testing of both glycerol and pentaerythritol monoesters so that their abiotic hydrolysis could be compared.
- Degradation should be demonstrated at relevant conditions and the OECD TG 111 hydrolysis study is conducted at a test concentration below the water solubility. Consequently, the test concentration is more environmentally relevant compared to ready biodegradation tests and allows an estimation of a half-life. However, according to ECHA's guidance (ECHA 2017b), the degradation half-lives obtained in a hydrolysis test cannot be compared to the persistence criteria of Annex XIII.
- The guidance also states that additional evidence is needed to examine whether the fate properties of the substance would cause attenuation of the hydrolysis rate in sediment or soil, or whether DOC would similarly affect the rate in aquatic media such as river or sea water. Additional studies, (e.g. examining the influence of DOC / adsorption processes on hydrolysis rates), may be necessary for this.

- Considering the issues above, degradation half-life below the P criteria in an OECD TG 111 hydrolysis study would not necessarily enable a 'not P/vP' conclusion.
- A similarity of abiotic hydrolysis of glycerol and pentaerythritol monoesters in an OECD TG 111 study may not be sufficient evidence for "not P/vP" as the fate properties of these monoesters may differ, which may affect their hydrolysis in environmentally relevant conditions.
- According to OECD TG 111, the study may be difficult to conduct with substances of minimal solubility in water. The pentaerythritol monoesters can be considered poorly water soluble on the basis of the QSAR predicted solubility.

ECHA notes that for the glycerol monoesters, the conclusion "not P/vP" could be drawn based on OECD TG 310 studies (together with other available data). The contribution of biodegradation to the observed degradation was essential, as indicated by the difference in primary degradation and ultimate degradation between the active tests and sterile controls. This suggests that a biodegradation study is needed also for the pentaerythritol monoesters to clarify the P/vP property.

In conclusion, ECHA does not see possibilities to conduct any testing which would represent a "lower tier" than the requested OECD TG 310 study and which could potentially rule out the P/vP concern e.g. by demonstrating that the primary degradation of the glycerol and pentaerytritol monoesters is similar as you suggested. Therefore, the OECD TG 310 request is maintained.

Regarding your proposed Tier 2, i.e., additional method development and feasibility studies, ECHA agrees that there are increased challenges in this study in comparison with the glycerol monoester studies. ECHA also agrees that the analytical method for analysing the substance and the degradation/transformation products needs development. ECHA notes that two different sterile controls are required and the analytical method should be validated separately for the sterile controls. ECHA considers that a feasibility study may be useful to identify and overcome challenges with the conduct of the studies and the analysis. The decision on whether to conduct a feasibility study/studies, as well as the content and extent of the potential feasibility studies, are left to your discretion. ECHA considers that it is difficult to determine beforehand whether the challenges (i.e. potential degradation of di-, tri- and tetraesters esters to monoesters and identification of the key

metabolites) are significantly higher than in the glycerol monoester study, as there is currently experimental information available only for the UVCB substance (ready biodegradability studies) but not for the primary or ultimate degradability of the different ester constituents.

In your comments you noted that interpretation of the ultimate degradation values is complicated further by the lower concentration of the key substance being assessed (monoesters) and presence of other constituents. You also asked on what basis or evidence ECHA has made its judgement that a 62% test concentration would be sufficient.

ECHA acknowledges that the expected lower monoester concentration (62 %w/w) in the test substance for the pentaerythritol monoester study is lower compared to the glycerol monoester studies (68-75 %w/w). ECHA notes that the CO_2 production and the concentrations of the monoesters and the other constituents and transformation products will be determined both in the active tests and in the sterile controls. From this information, the evaluating MSCA will be able to estimate the level of primary and ultimate degradation of the monoesters. The same methodology used in the assessment of the glycerol monoester studies can be applied. The uncertainty of extent of ultimate degradation of the monoesters may be higher for the pentaerythritol monoesters due to the lower concentration of the monoesters. However, ECHA considers that this does not significantly reduce the likelihood of obtaining valid results from the study because the key step is expected to be the primary transformation, which will be quantified based on the concentration measurements and comparison between active tests and the sterile controls. The uncertainty caused by the potential production of monoesters from the higher esters can be estimated based on decrease in concentrations of the higher ester, considering that per each molecule of the higher esters, one monoester molecule may be produced. ECHA further notes that another option would be to conduct a simulation study. However, similar uncertainties regarding quantification of biodegradation of the monoesters would occur in a simulation study, at least if conducted without radiolabeling, and the analytical methods would need to be more sensitive due to the lower test concentration. The ready biodegradation study is considered to be the most feasible as the first step to clarify the P/vP property, and may potentially avoid the need to conduct a simulation study.

Regarding your proposal to discuss the results and outcome of the feasibility study with ECHA before deciding if a full definitive study would still be required or whether this would be feasible, ECHA notes that the evaluating MSCA will be responsible for the assessment of the study. Therefore, discussion with the evaluating MSCA is possible before conducting the full OECD TG 310 study. Based on the currently available information, ECHA does not consider that the feasibility of conducting the definitive study should be discussed but the possible discussion would be on the technical aspects of the test design. ECHA also notes that in response to your comments, further considerations were added to the decision also to specify the circumstances when the measurements of the di-, tri-, and tetraesters and transformation products are not necessarily needed.

You indicated that you would like to proceed with this experimentation in a carefully considered way to ensure that any work can be correctly interpreted and does not lead to any further ambiguity or questions over the biodegradation potential of HRPE monoesters. ECHA fully agrees and considers that the test design described in the current decision is already a result of careful consideration, based on the available studies on the glycerol monoesters. As indicated above, you have the possibility to discuss with the evaluating MSCA regarding any further details of the test design.

d) Time needed to perform the requested studies

The deadline for provision of the requested data takes into account the standard deadline for performing an OECD TG 310 study (6 months) and includes the time required for developing an analytical method, conduct of the study, preparation of the study report and reporting in IUCLID. An additional 8 months is included since the duration of the test is extended by one month and time may be needed to manufacture the test substance, to develop analytical methods for transformation/degradation products, and since the test design is extended from the standard protocol, e.g., including primary degradation determination and two types of sterile controls. Furthermore, this additional time would allow the potential performance of a method development/feasibility study and potential discussion with the eMSCA regarding any further details of the test design.

In your comments you noted that this is not a standard study or standard test substance and that the test substance is not a commercially produced product. You considered that 8 months would not be sufficient to complete synthesis of the test substance, method

development/feasibility study and a definitive OECD TG 310 study, especially as the definitive study will be extended to 60 days. You proposed that a timeframe of 18 months would be required to complete these activities and report them sufficiently to ECHA. However, you did not provide any documentary evidence to justify why specifically 18 months would be necessary. Based on your comments, ECHA has reconsidered the time needed to fulfil the request and has changed the timeframe.

Therefore, ECHA considers that 14 months is a sufficient time for conduct and reporting of the requested study.

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

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U.S. EPA (2012). On-Line BIOWIN User's Guide (v4.10). Chapter 9.0. Available in EPI Suite v4.11 software.

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 follow up evaluation

- Due to initial grounds of concern for PBT/vPvB, the Member State Committee agreed to include the Substance (EC No 264-848-5, CAS No 64365-17-9) in the Community rolling action plan (CoRAP) to be evaluated in 2015. Finland is the competent authority ('the evaluating MSCA') appointed to carry out the evaluation.

- In accordance with Article 46(3) of REACH, the evaluating MSCA carried out its evaluation based on the information in the registration dossier(s) you submitted on the Substance on 29 May 2019 subsequent to a decision dated 7 February 2017, and on other relevant and available information.

- The evaluating MSCA completed its `follow up´evaluation considering that further information is required to clarify potential risk on PBT/vPvB.

- Therefore, it submitted a draft decision (Article 46(3) of REACH) to ECHA on 29 May 2020.

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.

(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 deadline

was amended.

Amendment of the deadline(s)

In your comments on the draft decision, you requested an extension of the timeline from 8 months as indicated in the draft decision to 18 months. Therefore, ECHA has partially granted the request and set the deadline to 14 months.

(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[8].

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, and
   - the following additional considerations:

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

The sample of the substance to be used shall represent the monoesterified pentaerythritol constituents of HRPE. The sample to be tested can be a fraction of the registered (UVCB) substance, or a specifically manufactured substance, consisting of monoesterified pentaerythritol constituents as far as technically possible. It is likely that the pentaerythritol monoesters of rosin acids may not be concentrated to the same purity as the respective glycerol monoesters which were tested in response to the first SEv decision. In your read-across justification report you have indicated that it has been possible to produce a sample containing 62% of the pentaerythritol monoesters.

It is the responsibility of all the Registrant(s) to agree on the test material and to document the necessary information on composition of the test material. The substance identity information of the registered substance and of the sample tested must enable the evaluating MSCA and ECHA to confirm the relevance of the testing for the substance subject to substance evaluation.

For the OECD TG 310 studies conducted on glycerol monoesters you have submitted composition data for test substances that were used for testing (the relative chromatogram peak areas of rosin acids, light ends, and tri-, di-, and monoesters of glycerol). You noted in your comments to the first SEv decision that, due to the complexity of the substance, further identification of the constituents in each group is impossible. ECHA considers that for the purpose of the present decision the concentrations of rosin acids, light ends, and tetra-, tri-, di-, and monoesters of pentaerythritol are necessary information. In addition, the concentrations of any other constituents or fractions of constituents that are present in concentrations equal to/above the above-mentioned fractions, or otherwise considered relevant for the purpose of the study by you, should be determined to the extent technically possible. ECHA acknowledges the analytical challenges due to the complexity of the substance and considers that further identification of the constituents within each of the above-mentioned fraction may be challenging.

The analytical techniques used shall have sufficient sensitivity to analyse and quantitate the monoesterified pentaerythritol constituents (and other relevant constituents and/or transformation products) for the purposes of the tests. In

practical terms, relevant constituents and transformation products need to be analysed to the extent technically possible. For example, in case that the results (e.g., gas chromatography/mass spectrometry (GC/MS) peaks) indicate differences in degradability of the different constituents within the monoester fraction, which could be important for the P/vP property, the degradation for the different constituents/subgroups of the monosters should be determined to the extent technically possible, to clarify the PBT/vPvB concern. ECHA notes that for the glycerol monoesters, two different groups of monoester, i.e, monoesters of dehydroabietic acid and monoesters of hydrogenated resin acids, were identified (based on GC/MS) in one of the OECD TG 310 studies (results presented in [redacted] (2017)), and differences were seen between the rates of degradation of these two groups of glycerol monoesters.

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/fractions of constituents (as specified in text above) of each Test Material and their concentration values and other parameters relevant for the property to be tested.

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

Technical instructions on how to report the above is available in the manual "How to prepare registration and PPORD dossiers"[9].

[9] https://echa.eu ropa.eu/manuals