Helsinki, 20 December 2016

Substance name: bis(2-ethylhexyl) 4,4'-{6-[4-tert-butylcarbamoyl) anilino]-1,3,5-triazine-2,4-diyldiimino}dibenzoate (hereafter called 'UVASORB HEB')
EC number: 421-450-8
CAS number: 154702-15-5
Date of Latest submission(s) considered[1]: 23 September 2016
Decision/annotation number: Please refer to the REACH-IT message which delivered this communication (in format SEV-D-XXXXXXXXXX-XX-XX/F)
Addressees: Registrant(s)[2] of bis(2-ethylhexyl) 4,4'-{6-[4-tert-butylcarbamoyl) anilino]-1,3,5-triazine-2,4-diyldiimino}dibenzoate (hereafter called the Registrant(s))

# DECISION ON SUBSTANCE EVALUATION

## 1. Requested information

Based on Article 46(1) of Regulation (EC) No 1907/2006 (the 'REACH Regulation'), you are requested to submit the following information on the registered substance:

1.1 **Sediment simulation testing (Aerobic and anaerobic transformation in aquatic sediment systems, EU C.24/OECD 308) using the registered substance (UVASORB HEB) at 20°C according to the specification of the test conditions listed in Appendix 1 Section 1.1.3.**

1.2 **Further information on uses and environmental emissions, as specified further in Appendix 1.**

You shall provide an update of the registration dossier(s) containing the requested information, including robust study summaries and, where relevant, an update of the Chemical Safety Report by **27 September 2018**. The deadline takes into account the time that the Registrants may need to agree on who is to perform any required tests.

The reasons of this decision are set out in Appendix 1. The procedural history is described in Appendix 2. Further information, observations and technical guidance as appropriate are provided in Appendix 3.

[1] This decision is based on the registration dossier(s) on the day until which the evaluating MSCA granted an extension for submitting dossier updates which it would take into consideration.

[2] The term Registrant(s), dossier(s) or registration(s) are used throughout the decision, irrespective of the number of registrants addressed by the decision.

## 2. Who performs the testing

Based on Article 53 of the REACH Regulation, you are requested to inform ECHA who will carry out the study on behalf of the other Registrant(s) within 90 days. Instructions on how to do this are provided in Appendix 3.

## 3. Appeal

This decision can be appealed to the Board of Appeal of ECHA within three months of its notification. An appeal, together with the grounds thereof, shall be submitted to ECHA in writing. An appeal has suspensive effect and is subject to a fee. Further details are described under http://echa.europa.eu/regulations/appeals.

Authorised[3] by Leena Ylä-Mononen, Director of Evaluation

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

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**Appendix 1: Reasons**

Based on the evaluation of all relevant information submitted on bis(2-ethylhexyl) 4,4'-{6-[4-tert-butylcarbamoyl) anilino]-1,3,5-triazine-2,4-diyldiimino}dibenzoate (hereafter: the registered substance or UVASORB HEB) and other relevant available information, ECHA concludes that further information is required in order to enable the evaluating Member State Competent Authority (MSCA) to complete the evaluation of whether the substance constitutes a risk to the environment. The evaluating MSCA will subsequently review the information submitted by you and evaluate if further information should be requested in order to clarify the concern for the strongly indicated formation of persistent or very persistent transformation products of the registered substance and further of their potential bioaccumulation and toxic effects.

Bis(2-ethylhexyl)4,4'-{6-[4-tert-butylcarbamoyl)anilino]-1,3,5-triazine-2,4-diyldiimino} dibenzoate (UVASORB HEB) was nominated for the CoRAP because it is fulfilling the screening criteria for persistence and bioaccumulation as defined in Annex XIII of the REACH Regulation.

All available data on persistence, bioaccumulation and toxicity were assessed in a weight-of-evidence approach including existing experimental data on bioaccumulation and toxicity of a structurally related analogue Ethylhexyltriazone ["Uvinul T150", CAS-Nr. 88122-99-0]. This assessment revealed sufficient evidence that the parent compound UVASORB HEB is not bioaccumulative or toxic.

However, as discussed below it is strongly indicated that UVASORB HEB could be biologically degraded to a certain degree and thus form metabolites. Based on QSAR estimates, some of the predicted metabolites screen as potentially persistent, bioaccumulative and toxic as defined under REACH Annex XIII.

## 1.1 Sediment simulation testing (Aerobic and anaerobic transformation in aquatic sediment systems, EU C.24/OECD 308) using UVASORB HEB at 20°C.

<u>The Concern(s) Identified and why new information is needed</u>

*1.1.1 PBT concern of possibly formed metabolites of UVASORB HEB*

UVASORB HEB is not readily biodegradable as shown by a screening test. In the screening tests according to OECD Test Guideline 301 B, 6 % degradation ($CO_2$-Evolution) was measured after 28 days of incubation. No transformation products were analytically determined in terms of this test on ready biodegradation. However, according to ECHA Guidance R.11 (version 2.0, November 2014) a negative result of a test on ready biodegradation (OECD 301 A-F) does not necessarily mean that the substance does not degrade or form transformation products under environmental conditions. The formation of $CO_2$ during this test indicates a certain degree of biologically derived degradation of UVASORB HEB to $CO_2$ in water in the presence of microorganisms.

Combining the information on biodegradation and structural aspects (ester and amide bonds) of UVASORB HEB, it is likely that UVASORB HEB is transformed in the environment to a certain degree. As UVASORB HEB is a large molecule, the degradation pathway is quite complex and may lead to the formation of complex metabolites. Only QSAR estimations describing the biodegradation pathway of the substance in the environment are available. The applied EAWAG Biocatalysis/ Biodegradation Prediction

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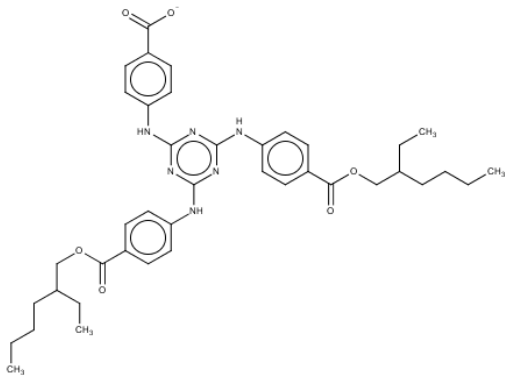
System[4] for the prediction of biodegradation pathways strongly indicates that several metabolites of UVASORB HEB are likely to be formed. Table 1 shows a range of possibly formed metabolites of UVASORB HEB having potential PBT properties, according to the screening criteria in REACH Guidance R11.

*Table 1: Chemical structure and QSAR estimations of possibly formed metabolites of UVASORB HEB regarding P, B and T screening information using COSMOmic 1504, EAWAG Pathway Prediction System, EPISuite, VEGA, T.E.S.T., and CHEMSPIDER.[5] $K_{lipw}$ = Membrane-Water-Partition-Coefficient, WS = water solubility.*

| Nr | Structure and SMILES code | Physicochemical properties and screening information on potentially P, B and T properties |
|---|---|---|
| 1 |  <br>SMILES:<br>CCCCC(CC)COC(=O)c1ccc(Nc2nc(Nc3ccc(cc3)C([O-])=O)nc(Nc3ccc(cc3)C(=O)OCC(CC)CCCC)n2)cc1 | Mol weight = 710.88 g/mol<br>Log $K_{oc}$ = 8.24, (pH sensitive, MCI, calculated)<br>Log $K_{ow}$ = **13.33**(calculated)<br>WS < 0.001 µg/L (calculated)<br>Log D(pH7) = **9.0** (calculated)<br>log $K_{lipw**}$ = **8.90** L/kg (calculated)<br>Dissociated fraction (pH 7): 99.6%<br><br>Hydrowin (pH 4/8): Half-life > 1 year<br><br>Biowin2 (non-linear model): 0.0139<br>Biowin3 (ultimate deg. time): 1.942<br>Biowin6 (MITI-non-lin.model): 0.0000<br>(Does not biodegrade fast/not ready biodegradable)<br><br>Estimated acute and chronic toxicity (Fish, Daphnia, Algae)<br><br>T.E.S.T: T potentially fulfilled<br>VEGA: T potentially fulfilled<br>ECOSAR: T not fulfilled<br><br>**Conclusion**<br>**P: potentially P/vP**<br>**B: potentially B/vB**<br>**T: potentially T** |

[4] http://eawag-bbd.ethz.ch/predict/ (accessed 15.07.2015)
[5] Note: The documentation of the QSAR results does not comply with REACH Annex XI, hence their reliability is limited.

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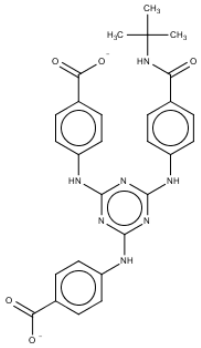
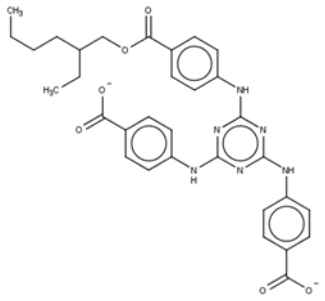
|---|---|---|
| 2 |  <br>SMILES:<br>CC(C)(C)NC(=O)c1ccc(Nc2nc(Nc3ccc(cc3)C([O-])=O)nc(Nc3ccc(cc3)C([O-])=O)n2)cc1 | Mol weight = 541.57 g/mol (estimated)<br>Log $K_{oc}$ = 5.76 (pH sensitive, MCI, calculated)<br>Log $K_{ow}$ = **6.60** (estimated)<br>WS= 0.89 µg/L (calculated)<br>Log D(pH7) = 0.9 (estimated)<br>log $K_{lipw}$ = **4.80** L/kg (estimated)<br><br>Dissociated fraction (pH 7): 99.0%<br><br>Hydrowin (pH 4/8): Half-life > 1 year<br><br>Biowin2 (non-linear model): 0.177<br>Biowin3 (ultimate deg. time): 1.26<br>Biowin6 (MITI-non-lin.model): 0.0000<br>(Does not biodegrade fast/not ready biodegradable)<br><br>Estimated acute and chronic toxicity (Fish, Daphnia, Algae)<br>T.E.S.T: T potentially fulfilled<br>VEGA: T potentially fulfilled<br>ECOSAR: T not fulfilled<br><br>**Conclusion**<br>**P: potentially P/vP**<br>**B: potentially B/vB**<br>**T: potentially T** |
| 3 |  <br>SMILES:<br>CCCCC(CC)COC(=O)c1ccc(Nc2nc(Nc3ccc(cc3)C([O-])=O)nc(Nc3ccc(cc3)C([O-])=O)n2)cc1 | Mol weight = 598.66 g/mol<br>Log $K_{oc}$ =7.48 (pH sensitive, MCI, calculated)Log $K_{ow}$ = **9.62** (calculated)<br>WS= 0.001 µg/L (calculated)<br>Log D(pH 7) = **5.0** (calculated)<br>log $K_{lipw}$ = **6.50** L/kg (calculated)<br>Dissociated fraction (pH 7): 99.2%<br><br>Hydrowin (pH 7): Half-life > 1 year<br><br>Biowin2 (non-linear model): 0.0021<br>Biowin3 (ultimate deg. time): 1.839<br>Biowin6 (MITI-non-lin.model): 0.0000<br>(Does not biodegrade fast/not ready biodegradable)<br><br>Estimated acute and chronic toxicity (Fish, Daphnia, Algae)<br>T.E.S.T: T potentially fulfilled<br>VEGA: T potentially fulfilled<br>ECOSAR: T not fulfilled<br><br>**Conclusion**<br>**P: potentially P/vP**<br>**B: potentially B/vB**<br>**T: potentially T** |

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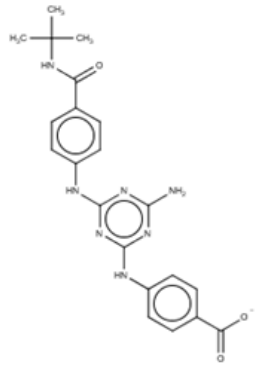
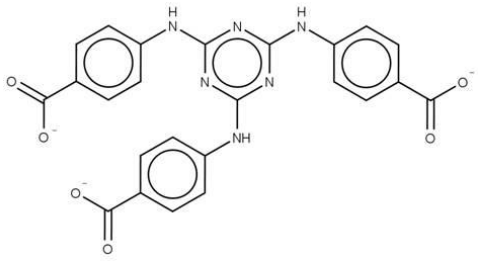
|---|---|---|
| 4 |  <br><br>SMILES:<br>CC(C)(C)NC(=O)c1ccc(Nc2nc(N)nc(Nc3ccc(cc3)C([O-])=O)n2)cc1 | Mol weight = 421.46 g/mol<br>Log $K_{oc}$ = 3.49(pH sensitive, MCI, calculated)<br>Log $K_{ow}$ = **4.50** (calculated)<br>Log D(pH 7) =1.4 (calculated)<br>WS= 0.0078 mg/L (calculated)<br>log $K_{lipw}$ = **4.1** L/kg (calculated)<br>Dissociated fraction (pH 7): 88.72%<br><br>Hydrowin (pH 7): Half-life > 1 year<br><br>Biowin2 (non-linear model): 0.000<br>Biowin3 (ultimate deg. time): 1.438<br>Biowin6 (MITI-non-lin.model): 0.0000<br>(Does not biodegrade fast/not ready biodegradable)<br><br>Estimated acute and chronic toxicity (Fish, Daphnia, Algae)<br>T.E.S.T: T potentially fulfilled<br>VEGA: T potentially fulfilled<br>ECOSAR: T not fulfilled<br><br>**Conclusion**<br>**P: potentially P/vP**<br>**B: potentially B/vB**<br>**T: potentially T** |
| 5 |  <br><br>SMILES:<br>[O-]C(=O)c1ccc(Nc2nc(Nc3ccc(cc3)C([O-])=O)nc(Nc3ccc(cc3)C([O-])=O)n2)cc1 | Mol weight = 486.45 g/mol<br>Log $K_{oc}$ = 6.70 (pH sensitive, MCI, calculated)<br>Log $K_{ow}$ = **5.91 ,** Log D(pH7) = -2.0(calculated)<br>WS= 0.0078 mg/L<br>log $K_{lipw}$ = **4.11** L/kg (calculated)<br>Dissociated Fraction (pH 7): 99.2%<br><br>Hydrowin: Half-life > 1 year<br><br>Biowin2 (non-linear model): 0.0003<br>Biowin3 (ultimate deg. time): 1.7371<br>Biowin6 (MITI-non-lin.model): 0.0000<br>(Does not biodegrade fast/not ready biodegradable)<br><br>Estimated acute and chronic toxicity (Fish, Daphnia, Algae)<br>T.E.S.T: T potentially fulfilled<br>VEGA: out of application domain<br>ECOSAR: T not fulfilled<br><br>**Conclusion**<br>**P: potentially P/vP**<br>**B: potentially B/vB**<br>**T: potentially T** |

No experimental data on the degradation of possibly formed metabolites of UVASORB HEB mentioned in Table 1 in soil, water or sediment are available. On the basis of QSAR estimations, metabolites mentioned in Table 1 are not ready biodegradable when applying BIOWIN 2/3 and 3/6 within EPISuite, Version 4.1 (Tab. 1). According to ECHA Guidance R.11, results obtained from biodegradation QSAR models are appropriate as screening information for the identification of potential P properties. Therefore, all of the possibly formed metabolites of UVASORB HEB indicated in Table 1 have to be regarded as potentially P/vP.

No experimental data are available regarding bioaccumulation and toxicity of possibly formed metabolites of UVASORB HEB. QSAR estimations (using EPISuite, OECD Toolbox, VEGA and T.E.S.T.) provided by the Registrant(s) and calculations performed by the evaluating MSCA indicate that some of the expected metabolites of UVASORB HEB (Table 1) are potentially bioaccumulative (calculated log $K_{ow}$> 4.5) and toxic (EC50 or LC50 < 0.1 mg/L/ NOEC<0.01 mg/L). Estimations using the model COSMOmic (Klamt et al. 2008) [6] point out that the main part of the possibly formed metabolites is expected to be ionized at pH value of 7 and thus very difficult to be assessed for bioaccumulative properties based on the current state of knowledge. Therefore, alternative parameters are needed instead of log $K_{ow}$ to assess the bioaccumulation potential of the ionized fraction of the metabolites. The membrane-water partition coefficient ($K_{lipw}$) has recently been proposed as rough indicator for the tendency of ionic or ionisable substances to partition into phospholipid membranes (Bittermann et al. 2014)[7]. Accordingly, the calculated phospholipid-water partition coefficients point out that some of the possibly formed ionised metabolites of UVASORB HEB will tend to sorb on phospholipid membranes indicating a certain potential for bioaccumulation. Nonetheless, some metabolites are predicted to have non-ionic fractions at environmentally relevant pH values. The log $K_{ow}$ values > 4.5 of these non-ionic fractions further indicate an increased bioaccumulation potential of the possibly formed metabolites of UVASORB HEB. According to ECHA Guidance R.11 (2014), results obtained from calculated log $K_{ow}$ values and other suitable or reliable information are appropriate as screening information for the identification of potentially B/vB and T properties. Therefore, according to calculated log $K_{ow}$ and log $K_{lipw}$ values, as well as QSAR estimations on toxicity, all of the possibly formed metabolites of UVASORB HEB mentioned in Table 1 have potential B/vB and T properties.

Even if the parent compound is supposed to be not PBT itself, possibly formed metabolites of UVASORB HEB have potential PBT/vPvB properties. Therefore, the PBT concern is related to the metabolites of UVASORB HEB. Thus, it is necessary to further explore the degradation behaviour to enable the determination of degradation pathways of UVASORB HEB with regard to the formation of metabolites and the determination of their concentrations in the test system under environmentally relevant conditions.

*1.1.2 Determination of the most relevant compartment for simulation testing*

The determination of the most relevant environmental compartment for simulation testing depends on the use of UVASORB HEB, its physico chemical properties as well as

[6] Klamt, A. et al 2008: COSMOmic: a mechanistic approach to the calculation of membrane-water partition coefficients and internal distributions within membranes and micelles. J. Phys.Chem B. 112(38), pp. 12148 – 12157.

7 Bittermann, K. et al. 2014: Prediction of Phospholipid-Water Partition Coefficients of Ionic Organic Chemicals Using the Mechanistic Model COSMOmic. J. Phys. Chem. B. 118(51), pp 14833 –14842.

its distribution in different environmental compartments.

According to the Mackay level III model, the aquatic and soil compartments are considered as relevant, whereas low amounts of UVASORB HEB tend to volatise to air or distribute to the sediment (Table 2).

*Table 2: Relative mass distribution (%) of UVASORB HEB according to the Mackay level III (steady state) model of EpiSuite v. 4.1*

| Compartment | Mass distribution (%) |
|---|---|
| Air | 0.000752 |
| Water | 4.02 |
| Soil | 95.9 |
| Sediment | 0.0835 |

According to the STP (Sewage treatment plant) model, most of UVASORB HEB will be adsorbed to sludge (Table 3). The fraction adsorbed to STP sludge is normally assumed to be disposed of on soil and hence 93.26 % of UVASORB HEB is assumed to expose the soil compartment. A relevant fraction of 5.96 % will not be removed in the STP and will enter the aquatic environment. Only minor amounts of UVASORB HEB (0.78 %) will be degraded in the STP.

*Table 3: Relative mass distribution (%) of UVASORB HEB according to the STP model of EpiSuite v. 4.1*

| Removal In Wastewater Treatment: | Mass distribution (%) |
|---|---|
| Total removal: | 94.04 |
| Total biodegradation: | 0.78 |
| Total sludge adsorption (potentially deposed of on soil): | 93.26 |
| Total to Air: | 0.00 |
| Not removed in the STP, i.e. released to surface water | 5.96 |

UVA SORB HEB is used as UV-A filter in personal care products. According to the use profile of the substance, emission to the environment will be occurring directly by people e.g. swimming in surface water and indirectly to waste water discharges of showering or bathing that drain to STP. UVASORB HEB has a high adsorption potential (Log $K_{oc}$ 5.63) to soil/ sediment and a low water solubility (<0.00075 mg/L). When emitted directly or to the aquatic environment, UVASORB HEB will mainly distribute to the sediment compartment due to its adsorption i) directly to the sediment or ii) indirectly to particulate matter in the surface water which will become part of the sediment due to sedimentation. In STPs a large fraction of the substance may be adsorbed to STP sludge which may be deposited on soil. The fraction not adsorbed to STP sludge will be released to surface water probably mainly adsorbed to particulate matter emitted from the STP.

On the basis of the modelling results a significant extent of UVASORB HEB will be distributed to the aquatic and the soil compartment mainly depending on the extent of STP sludge deposition over soil. With regard to its high adsorption potential it is assumed that UVASORB HEB will mainly be distributed to the sediment compartment, when emitted to the aquatic environment, and only minor parts will remain in the aquatic phase. Therefore, soil and sediment is regarded as relevant compartment for simulation

testing of UVASORB HEB. However, one simulation test will be sufficient to assess the degradation pathway of UVASORB HEB under environmentally relevant conditions and to identify possibly formed metabolites of UVASORB HEB. Thus, only sediment simulation testing using UVASORB HEB at 20°C is requested.

*1.1.3 Specification of the test conditions*

The requested simulation study on degradation of UVASORB HEB in sediment should enable i) the determination of degradation pathways of UVASORB HEB in sediment with regard to the formation of metabolites and ii) the identification of formed metabolites of UVASORB HEB. The OECD 308 simulation test should be performed using $^{14}$C-radiolabelled UVASORB HEB. The radiolabel should be located in most stable part of the molecule, thus the 1,3,5-triazine ring. Radiolabelling of the most stable part of the molecule is necessary for identification of transformation products relevant for PBT assessment (at a concentration of ≥ 0.1 % w/w unless it can be demonstrated that this is technically not possible). The test set-up shall enable to perform a mass balance. During the test duration, transformation products of UVASORB HEB should be analysed by means of the $^{14}$C-radiolabel. UVASORB HEB should be added in a concentration appropriate to successfully identify possibly formed metabolites. Due to its low water solubility (<0.00075 mg/L), UVASORB HEB should be added directly to the sediment by use of a solvent.
According to the test on ready biodegradation, UVASORB HEB degrades slowly. To maximize the probability for the formation and identification of metabolites of UVASORB HEB in the requested OECD 308 test, a temperature of 20°C has been selected.

Alternative approaches and Proportionality of the request

The request for the sediment simulation testing using UVASorb HEB at 20°C is suitable and necessary to obtain information on the degradation pathway of UVASORB HEB and will allow clarifying whether metabolites of UVASORB HEB having potentially PBT/vPvB properties are formed under environmental relevant conditions. More explicitly, there is no suitable alternative approach to obtain similar information imposing a lesser burden to the Registrant(s).

If the attained data confirm that potential PBT/vPvB metabolites of UVASORB HEB are formed, an analysis of risk management options will be carried out taking into account information on use and exposure. Potential options are the inclusion in the Candidate List and subsequent Authorisation, but also Restriction and Harmonized C&L.

Comments from the Registrant(s) on the original draft decision

In their comments on the draft decision the Registrant(s) challenge the water solubility of 0.00075 mg/ L used by the evaluating MSCA and suggests using a water solubility of 0.005 mg/ L. ECHA does not follow this proposal as two endpoint study records were submitted within the registrations. One study (dated 2008) was conducted according to OECD 105 / A.5 EU method with the column elution method. A water solubility of < 0.00075 mg/l resulted. The second endpoint study (dated 1996) was conducted with the flask method. A water solubility of 0.005 mg/l (T=20 °C; pH-value: unknown) resulted. The method used in the second endpoint study record (flask method) is not valid for the following reason: in the "Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.7a: Endpoint specific guidance [Version 4.1, October 2015]" in table R.7.1-5 "Test methods for the determination of water solubility" is affecting on

both methods and their application range. The column elution method is suitable for low water solubilities (< $10^{-2}$ g/l). For the flask method it has to be distinguished between the application area of fast stirring techniques (300 – 400 rpm) which is suitable for higher solubilities and the application field of slow-stirring techniques (<100 rpm) for lower solubilities (Letinski et al, 2002[8]). The slow-stirring method was developed after 1996. Therefore the submitted test using the flask method has to be assessed as non-valid. Therefore, the water solubility of the substance has to be recorded with < 0.00075 mg/l (T=20°C, pH-value = 5.4 - 7.1) as this result was gained with a valid test.

Another comment of the Registrant(s) is that the substance may however also be degraded by abiotic processes that are relevant under environmental conditions (phototransformation). ECHA disagrees with the suggestion to test the transformation products stepwise in dependence of QSAR calculations. According to the requested OECD 309 simulation study one or two sterile control flasks have to be prepared for the purpose of interpretation and quantification of abiotic degradation processes of the test substance possibly occurring during the incubation. However, the contribution of photo degradation in water to persistence in the environment is significant only for substances that reside in water to a considerable extent (Jimenez and van de Meent, 2011[9]). Due to its high log Koc value of 5.63, UVASORB HEB is expected to be distributed in soil and sediment and it is expected that less amounts of the substance remain in the water phase. Therefore, photo degradation plays a minor role regarding the persistency of the substance in the environment.

A further comment of the Registrant(s) is that the transformation products, which appear to increase in concentration during the course of the study, should be identified unless it can be demonstrated that this cannot be achieved with reasonable efforts. ECHA disagrees to only identify transformation products that increase in concentration during the OECD 309 simulation test because some of the potential PBT/vPvB transformation products may be formed very fast to a maximum content and then their concentrations i) remain static or ii) slowly decrease in the test system in course of time. Furthermore, according to ECHA's Guidance on Information Requirements and Chemical Safety Assessment R. 11 (2014) in general transformation products detected at ≥ 10% of the applied radioactivity in the total test system at any sampling time should be identified unless reasonably justified otherwise. Transformation products for which concentrations continuously increase during the study should also be considered for identification, even if their concentrations do not exceed the limits of 10% as this may indicate persistence.

The Registrant(s) suggest conducting long-term toxicity studies to aquatic organisms initially on aged aqueous solutions of the substance, and only in the event that these studies demonstrate chronic toxicity, there is a requirement to conduct the simulation testing. ECHA disagrees with this approach as toxicity tests with aged solution would not allow assessing which of the transformation products, in case several are formed, has an effect on the test organism. Consequently, it would not be possible to assign a NOEC or an EC50 to any of the individual transformation products. This would thus result in unnecessary animal testing.

Studies performed according to OECD guidelines 211 (Daphnia magna reproduction test)

[8] Letinski, D. J., Connelly, M. J., Peterson, D. R., & Parkerton, T. F. (2002). Slow-stir water solubility measurements of selected alcohols and diesters. *Chemosphere*, *48*(3), 257-265.

[9] Castro Jiménez J and Van de Meent D (2011). Accounting for photodegradation in P-assessment of chemicals. Radboud University Nijmegen. Reports Environmental Science no 381, 2011.

and 210 (fish early life stage toxicity test) appear appropriate by ECHA. The first step in a PBT assessment for metabolites should be determination of their degradation half-life. If the metabolites are long-lived or persistent, they should then be assessed for bioaccumulation and toxicity. Hence, it does not seem justified to conduct the toxicity tests first.

Assessment of the proposal for amendments (PfAs) and the Registrant(s)' comments on them

A proposal for amendment (PfA) was received suggesting a request of an OECD 308 test instead of the OECD 309 test. Another PfA expressed that a marine testing system is not appropriate for the use pattern, and further pointed out that the compound is expected to rapidly partition out of the water, making sediment or sewage sludge a more appropriate exposure route. The evaluating MSCA reviewed the proposals for amendment received and amended the draft decision accordingly.

Furthermore, another PfA suggested that it should be more explicitly demonstrated which relevant metabolites of UVASORB HEB having potentially PBT/vPvB properties are expected to be formed. The evaluating MSCA reviewed the proposals for amendment received and amended the draft decision accordingly by inserting a table indicating relevant metabolites and QSAR estimates for these metabolites respectively regarding their PBT properties under Appendix 1.

The Registrant(s) agree that, based on the expected exposure profile, the OECD 308 test (water/sediment study) will be a more realistic test compared to the requested OECD 309 test.

The Registrant(s) also agree that the purpose of the test is to assess the metabolism of the registered substance and experimentally determine the metabolites formed.

The Registrant(s) point out that there is no need to further pursue quantitative degradation data on the parent substance in order to examine the P criterion (i.e. it is already established via the B criterion that the parent substance is not PBT or vPvB). ECHA agrees that the PBT concern is related not to the parent but to the metabolites. ECHA agrees that there is no need to obtain a degradation half-life for the parent compound as the parent is identified as non-PBT. However, there is a need to further explore the degradation behavior to enable the determination of degradation pathways of UVASORB HEB with regard to the formation of metabolites and the determination of their concentrations in the test system under environmental relevant conditions.

In the course of the second commenting by the Registrant(s) regarding the PfAs, the Registrant(s) submitted again two documents containing a PBT-assessment of the parent UVASORB HEB and of the possibly formed metabolites. These documents are the same as had been already submitted by the Registrants(s) to the evaluating MSCA in September 2015. Hence, the submitted data had been examined in detail and considered by the evaluating MSCA and ECHA for the PBT- assessment and for the final conclusion regarding potential PBT metabolites.

The PBT-assessment provided by the Registrant(s) is based solely on QSAR data using the software EAWAG prediction model, the OECD Toolbox, VEGA, T.E.S.T. All twelve metabolites indicated by the Registrant(s) in the PBT-assessment were also assessed by the evaluating MSCA. According to the EAWAG prediction model and depending on the

degree of degradation also other metabolites than indicated by the Registrants(s) were identified by the evaluating MSCA. Metabolites number 1, 3, and 5 indicated in Table 1 of this decision which show a certain potential for PBT properties, were the same as predicted by the Registrant(s). The Registrant(s) come to the conclusion in the PBT assessment that even the main part of the metabolites is predicted to be P/vP, B/vB and T, no PBT concern arises from the metabolites because some of the predicted BCF values are below the B trigger of 2000. The conclusion stated by the Registrant(s) that no PBT concern arises from the metabolites is based on the assumption that "the estimation of metabolites is theoretical and that as the substance is predicted not to readily degrade and its bioavailability will be limited by its sorption behavior, formation of metabolites is unlikely to occur in high quantities."

ECHA disagrees with this argumentation as some of the metabolites are definitely PBT on the screening level and other metabolites than indicated by the Registrant(s) may be formed. As it is established that QSAR prediction may suffer from great uncertainties information based on QSAR calculations shall be used only as part of an overall weight-of-evidence approach beside other available information from testing and non-testing data. Therefore, further experimental data are needed to finally clarify the PBT concern of the metabolites.

Another PfA suggested performing the requested simulation test at a temperature of 20°C instead of 12°C and 25°C. The evaluating MSCA reviewed the proposals for amendment received and amended the draft decision accordingly.

In their comments on this PfA on the original draft decision the Registrant(s) agree to the PfA that the PBT concern is addressed to metabolites and not to parent. On this basis the Registrant(s) suggest that the higher study temperature is appropriate to form more metabolites. However, the Registrant(s) consider that this would also be expected to increase the subsequent degradation rate of the metabolites and hence appears to make the results less suited to the stated aim of determining whether the metabolites are "persistent" or not. Furthermore, the Registrant(s) support ECHA's view that marine water is of questionable significance and proposes the test to be undertaken in surface water.

The Registrant disagreed with a PfA made on the originally requested OECD 309 test which proposed to identify metabolites to a concentration of 0.1% w/w in that study. The Registrants provided several reasons to argue that this is not reasonable or practical. ECHA notes that these comments refer to the OECD 309 test method which was originally proposed. ECHA considers that for the OECD 308 test which is now requested, the appropriate threshold for identification of the transformation products is specified in paragraph 41 of the test guideline.

Another PfA suggested performing an OECD 301/306 test instead of the requested OECD 309 test. The evaluating MSCA disagreed to this PfA and did not change the draft decision for the following reasons: OECD 301 tests are artificial and do not simulate realistic environmental conditions for degradation processes of a substance due to their high inoculum density and high test concentration. In the available test on ready biodegradability of UVASORB HEB, 6% degradation after 28 days ($CO_2$-evolution) was observed indicating that biodegradation of UVASORB HEB in aqueous test systems is a slow process. Thus, it is assumed that the metabolites in the OECD 301 test using radio labelled UVASORB HEB are also formed very slowly and thus the probability and feasibility of the identification of slowly formed metabolites of UVASORB HEB in OECD

301 test is limited.

According to the use and applications of UVASORB HEB, the aquatic environment will likely be exposed to the substance. Due to its high log Koc value (Log Koc 5.63), UVASORB HEB is expected to dissipate to the sediment and only minor parts of the substance remain in the water phase. Therefore, test conditions of OECD 308 seem to be more realistic to investigate the substance's degradation pathways compared to OECD 306 test. In addition, in order to obtain information on the degradation pathway, data on metabolites are needed which requires a sufficient number of microorganisms in the inoculum. OECD 308 will provide a higher number of microorganisms compared to OECD 306 and thus it is more likely to generate the data needed by using OECD 308. Furthermore, as it is unknown at which point in time degradation will occur, it seems reasonable to use a test that lasts long. In this respect an OECD 308 test is more favourable than an OECD 306 test because test duration in the OECD 308 guideline is 100 days whereas it is only 60 days provided that the Shake flask Method of OECD 306 is used.

The OECD 306 test uses natural seawater for the inoculum, but the standard test concentration of this test is unrealistically high (2 mg/l; Closed Bottle method) compared to the low water solubility of UVASORB HEB. For the investigation of degradation pathways of compounds at environmentally realistic concentrations, the use of radio labelled test compounds is needed (OECD 306). However, performing an OECD 306 test would still be challenging despite the use of radio labelled compounds because of the low water solubility of UVASORB HEB (0.00075 mg/l).

In their comments the Registrant(s) disagree on the PfA to conduct OECD 301 or OECD 306 studies (radiolabelled) prior to, or instead of, the current OECD 309 proposal. The Registrant(s) state that the reasons for this PfA are not entirely clear. The results of the study are likely to be subject to interpretation and may well result in the OECD 309 study being required anyway. Therefore, the Registrant(s) see no advantage in this proposal.

Conclusion

Therefore, based on the substance evaluation and pursuant to Article 46(1) of the REACH Regulation, ECHA concludes that you are required to carry out the following study using the registered substance subject to this decision: Sediment simulation testing (Aerobic and anaerobic transformation in aquatic sediment systems, EU C.24/OECD 308) using UVASORB HEB at 20°C. Testing should be at a concentration enabling successful identification/ characterization and quantification of possibly formed metabolites of UVASORB HEB in the sediment system.

If, based on the outcome of the above requested sediment simulation test, the Registrant(s) identify metabolites of UVASORB HEB which have potential PBT/vPvB properties, these metabolites have to be regarded as relevant. According to REACH Annex XIII the identification of PBT/vPvB substances should also take account of the PBT/vPvP properties of relevant transformation and/or degradation products.

The further testing procedure of UVASORB HEB will depend upon which transformation products are generated. If demonstrably no transformation products are formed in the requested OECD 308 study, the substance is not subject to degradation, and hence, no further testing of potential metabolites might be necessary. In contrast, if transformation products are formed during the OECD 308 study using $^{14}$C-radiolabelled UVASORB HEB

which have potential PBT or vPvB properties, further information on persistence, bioaccumulation and toxicity of the identified transformation products might be needed.

### *1.2* Further information on uses and environmental emissions

The Concern(s) Identified and why new information is needed

UVASORB HEB is used as UV-Filter in personal care products and is expected to enter the environment via waste water, direct discharges or directly into swimming waters. Due to insufficient information regarding environmental release estimation, it is not possible to quantify possible risks for the environment from manufacture, formulation and uses of UVASORB HEB.

It must be noted that the registration documents do not contain an exposure assessment. UVASORB HEB is currently not (self)-classified as hazardous under the CLP regulation. Therefore, taking into account the potential PBT or vPvB properties of possibly formed metabolites of UVASORB HEB, and the wide dispersive use of consumer products containing UVASORB HEB, information on its uses and their associated environmental emissions is required. If the registered substance is identified as PBT or vPvB, this information will be used for choosing the most appropriate risk management option for UVASORB HEB.

Conclusion

Therefore, based on the substance evaluation and pursuant to Article 46(1) of the REACH Regulation, ECHA concludes that you are required to provide the following information on the registered substance subject to this decision: Further information on uses and environmental emissions.

## Appendix 2: Procedural history

On the basis of an opinion of the ECHA Member State Committee and due to initial grounds for concern relating to PBT and vPvB, Bis(2-ethylhexyl) 4,4'-{6-[4-tert-butylcarbamoyl)anilino]-1,3,5-triazine-2,4-diyldiimino}dibenzoate (UVASORB HEB), CAS No 154702-15-5 (EC No 421-450-8) was included in the Community rolling action plan (CoRAP) for substance evaluation to be evaluated in 2015. The updated CoRAP was published on the ECHA website on 17 March 2015. The Competent Authority of Germany (hereafter called the evaluating MSCA) was appointed to carry out the evaluation.

Pursuant to Article 45(4) of the REACH Regulation the evaluating MSCA carried out the evaluation of the above substance based on registration(s) submitted by you and the other Registrant(s) and other relevant and available information.

The evaluating MSCA considered that further information was required to clarify the abovementioned concerns. Therefore, it prepared a draft decision pursuant to Article 46(1) of the REACH Regulation to request further information. It submitted the draft decision to ECHA on 17 March 2016.

The decision making followed the procedure of Articles 50 and 52 of the REACH Regulation.

ECHA notified you of the draft decision and invited you and the other Registrant(s) to provide comments.

### Registrant(s)' commenting phase

ECHA received comments from you and forwarded them to the evaluating MSCA without delay.

The evaluating MSCA took into account the comments from you, which were sent within the commenting period, and they are reflected in the Reasons (Appendix 1).

### Proposals for amendment by other MSCAs and ECHA and referral to 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.

Subsequently, the evaluating MSCA received proposal(s) for amendment to the draft decision and modified the draft decision. They are reflected in the Reasons (Appendix 1).

ECHA referred the draft decision, together with your comments, to the Member State Committee.

ECHA invited you to comment on the proposed amendment(s). Any comments on the proposal(s) for amendment were taken into account by the Member State Committee and are reflected in the Reasons (Appendix 1).

A unanimous agreement of the Member State Committee on the draft decision was reached on 10 October 2016 in a written procedure launched on 30 September 2016 and ECHA took the decision according to Article 51(6) of the REACH Regulation.

## Appendix 3: Further information, observations and technical guidance

1. This decision does not imply that the information provided by you in the registration(s) is in compliance with the REACH requirements. The decision neither prevents ECHA from initiating compliance checks on your dossier(s) at a later stage, nor does it prevent a subsequent decision under the current substance evaluation or a new substance evaluation process once the present substance evaluation has been completed.

2. Failure to comply with the request(s) in this decision, or to fulfil otherwise the information requirement(s) with a valid and documented adaptation, will result in a notification to the enforcement authorities of your Member State.

3. In relation to the required experimental stud(y/ies), the sample of the substance to be used shall have a composition that is within the specifications of the substance composition that are given by all Registrant(s). It is the responsibility of all the Registrant(s) to agree on the tested material to be subjected to the test(s) subject to this decision 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.

4. In relation to the experimental stud(y/ies) the legal text foresees the sharing of information and costs between Registrant(s) (Article 53 of the REACH Regulation). You are therefore required to make every effort to reach an agreement regarding each experimental study for every endpoint as to who is to carry out the study on behalf of the other Registrant(s) and to inform ECHA accordingly within 90 days from the date of this decision under Article 53(1) of the REACH Regulation. This information should be submitted to ECHA using the following form stating the decision number above at:
https://comments.echa.europa.eu/comments_cms/SEDraftDecisionComments.aspx

   Further advice can be found at
http://echa.europa.eu/regulations/reach/registration/data-sharing . If ECHA is not informed of such agreement within 90 days, it will designate one of the Registrants to perform the stud(y/ies) on behalf of all of them.