SUBSTANCE EVALUATION CONCLUSION

as required by REACH Article 48

and

EVALUATION REPORT

for

bis(2-ethylhexyl) 4,4'-{6-[4-tert-butylcarbamoyl) anilino]-1,3,5-triazine-2,4-diyldiimino} dibenzoate

EC No. 421-450-8

CAS RN 154702-15-5

Evaluating Member State(s): Germany

Dated: 5 April 2023

Evaluating Member State Competent Authority

BAuA
Federal Institute for Occupational Safety and Health
Division 5 - Federal Office for Chemicals
Friedrich-Henkel-Weg 1-25
D-44149 Dortmund, Germany

Year of evaluation in CoRAP: 2015

Before concluding the substance evaluation, a Decision to request further information was issued on: 20 December 2016
Member State concluded the evaluation without any further need to ask more information from the registrants under Article 46(1) decision.

Further information on registered substances here:

http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances

DISCLAIMER

This document has been prepared by the evaluating Member State as a part of the substance evaluation process under the REACH Regulation (EC) No 1907/2006. The information and views set out in this document are those of the author and do not necessarily reflect the position or opinion of the European Chemicals Agency or other Member States. The Agency does not guarantee the accuracy of the information included in the document. Neither the Agency nor the evaluating Member State nor any person acting on either of their behalves may be held liable for the use which may be made of the information contained therein. Statements made or information contained in the document are without prejudice to any further regulatory work that the Agency or Member States may initiate at a later stage.

Foreword

Substance evaluation is an evaluation process under REACH Regulation (EC) No. 1907/2006. Under this process the Member States perform the evaluation and ECHA secretariat coordinates the work. The Community rolling action plan (CoRAP) of substances subject to evaluation, is updated and published annually on the ECHA web site[1].

Substance evaluation is a concern driven process, which aims to clarify whether a substance constitutes a risk to human health or the environment. Member States evaluate assigned substances in the CoRAP with the objective to clarify the potential concern and, if necessary, to request further information from the registrant(s) concerning the substance. If the evaluating Member State concludes that no further information needs to be requested, the substance evaluation is completed. If additional information is required, this is sought by the evaluating Member State. The evaluating Member State then draws conclusions on how to use the existing and obtained information for the safe use of the substance.

This Conclusion document, as required by Article 48 of the REACH Regulation, provides the final outcome of the Substance Evaluation carried out by the evaluating Member State. The document consists of two parts i.e. A) the conclusion and B) the evaluation report. In the conclusion part A, the evaluating Member State considers how the information on the substance can be used for the purposes of regulatory risk management such as identification of substances of very high concern (SVHC), restriction and/or classification and labelling. In the evaluation report part B, the document provides explanation how the evaluating Member State assessed and drew the conclusions from the information available.

With this Conclusion document the substance evaluation process is finished and the Commission, the Registrant(s) of the substance and the Competent Authorities of the other Member States are informed of the considerations of the evaluating Member State. In case the evaluating Member State proposes further regulatory risk management measures, this document shall not be considered initiating those other measures or processes. Further analyses may need to be performed which may change the proposed regulatory measures in this document. Since this document only reflects the views of the evaluating Member State, it does not preclude other Member States or the European Commission from initiating regulatory risk management measures which they deem appropriate.

[1] http://echa.europa.eu/regulations/reach/evaluation/substance-evaluation/community-rolling-action-plan

Contents

Part A. Conclusion

1. CONCERN(S) SUBJECT TO EVALUATION

Bis(2-ethylhexyl) 4,4'-{6-[4-tert-butylcarbamoyl) anilino]-1,3,5-triazine-2,4-diyldiimino} dibenzoate (UVASorb HEB, "the Substance") was originally selected for substance evaluation to clarify concerns about:

- suspected PBT/vPvB properties
- wide dispersive use
- exposure of the environment

No further concerns were identified during the evaluation.

2. OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

ECHA has opened and as of 7 May 2021 concluded two targeted compliance checks on the Substance without a decision for further standard information requirements being issued.[2]

3. CONCLUSION OF SUBSTANCE EVALUATION

The evaluation of the available information on the substance has led the evaluating Member State to the following conclusions, as summarised in the table below.

Table 1

CONCLUSION OF SUBSTANCE EVALUATION	
Conclusions	**Tick box**
Need for follow-up regulatory action at EU level	
Harmonised Classification and Labelling	
Identification as SVHC (authorisation)	
Restrictions	
Other EU-wide measures	
No need for regulatory follow-up action at EU level	x

[2] https://echa.europa.eu/de/information-on-chemicals/dossier-evaluation-status/-/dislist/substance/100.102.002

4. FOLLOW-UP AT EU LEVEL

4.1. Need for follow-up regulatory action at EU level

The eMSCA does not foresee the need for further regulatory measures.

4.1.1. Harmonised Classification and Labelling

Not applicable.

4.1.2. Identification as a substance of very high concern, SVHC (first step towards authorisation)

Based on the new information generated via the substance evaluation procedure, the Substance – while being very persistent – does not fulfil the criteria for PBT or vPvB according to Annex XIII REACH. Hence, the Substance is not a candidate for identification as an SVHC according to Article 57.

4.1.3. Restriction

Not applicable.

4.1.4. Other EU-wide regulatory risk management measures

Not applicable.

5. CURRENTLY NO FOLLOW-UP FORESEEN AT EU LEVEL

5.1. No need for regulatory follow-up at EU level

Table 2

REASON FOR REMOVED CONCERN The concern could be removed because	Tick box
Clarification of hazard properties/exposure *Based on the available information, the Substance is very persistent but does not fulfil the criteria for bioaccumulation or toxicity according to Annex XIII REACH.*	x
Actions by the registrants to ensure safety, as reflected in the registration dossiers (e.g., change in supported uses, applied risk management measures, etc.)	

5.2. Other actions

Not applicable.

6. TENTATIVE PLAN FOR FOLLOW-UP ACTIONS (IF NECESSARY)

Not applicable.

Part B. Substance evaluation

7. EVALUATION REPORT

7.1. Overview of the substance evaluation performed

The Substance was originally selected for substance evaluation to clarify concerns about:

- suspected PBT/vPvB properties
- wide dispersive use
- exposure of the environment

No further concerns were identified during the evaluation.

Table 3

EVALUATED ENDPOINTS	
Endpoint evaluated	**Outcome / conclusion**
Persistence	Concern confirmed. Based on simulation data in sediment generated during the substance evaluation, the Substance is very persistent (vP) according to Annex XIII REACH.
Bioaccumulation	Concern unresolved. The high hydrophobicity of the Substance raises a concern for slow bioaccumulation which however cannot be investigated further with existing validated methods. Based on the currently available PBT guidance and the available data, the eMSCA concludes that the B/vB criterion is likely not fulfilled.
Toxicity	No concern. The Substance does not screen as toxic (T) according to Annex XIII. Based on available information, the eMSCA concludes that the T criterion is likely not fulfilled for the Substance.
PBT/vPvB	Concern unresolved. According to the assessment of the eMSCA, the Substance is likely neither a PBT nor a vPvB substance. Remaining concerns about a slow bioaccumulation potential cannot be investigated further based on validated testing methods and existing PBT guidance. The formation of potential PBT/vPvB metabolites / transformation products is not expected, as no transformation products were observed in the available biodegradation test.
Wide dispersive use	Concern confirmed. The Substance is used as an UV filter in cosmetics (i.e., sunscreen products). Therefore, wide dispersive of UVASorb HEB occurs.
Exposure of the environment	Concern confirmed. As the Substance is not classified, no environmental exposure assessment has been provided in the registration dossiers. However, through its main use, direct exposure of environmental compartments via washing off the applied sunscreen products in surface waters during swimming or indirect exposure via wastewater or sewage sludge application to soil can be assumed.

7.2. Procedure

The evaluation of the PBT properties of the Substance was carried out from May to September 2015 based on the registration dossiers update from November 2012. Furthermore, an updated PBT assessment which was provided in September 2015 by the Registrant(s) was considered in the evaluation process. The updated PBT assessment includes new QSAR estimations (using EPISuite, QSAR toolbox, T.E.S.T. and VEGA) for the parent compound and likely formed metabolites concerning their P, B and T properties, respectively.

The Substance fulfils the screening criteria for PBT and vPvB substances according to Annex XIII of the REACH regulation. Accordingly, the substance evaluation was targeted to the persistency, the bioaccumulation potential and toxicity. As the T criterion is based on an aquatic NOEC for pelagic organisms, the terrestrial compartment and terrestrial toxicity was not subject of this substance evaluation. Additional information from literature regarding PBT properties and the environmental behaviour of adequate read-across candidates were reviewed for the evaluation process. A literature search was performed prior to the assessment including monitoring data but did not reveal additional information beyond those found in the registration dossier.

Regarding the exposure, it must be noted that the registration documents do not contain an exposure assessment. The Substance is currently not (self)-classified as hazardous under the CLP regulation. Therefore, an exposure assessment and an environmental risk characterisation are not required.

The eMSCA submitted a draft decision with further information requirements regarding biodegradation in sediment and uses and environmental emissions to ECHA. Following the decision-making procedure, a substance evaluation decision with further information requirements was taken by ECHA on 20 December 2016.[3] The decision was appealed before the Board of Appeal (BoA) of ECHA. In its decision from 15 January 2019, the BoA partially annulled the substance evaluation decision and removed the previously included information requirement on uses and environmental emissions.[4] An action against the decision of the BoA before the European General Court was dismissed on 16 December 2020.[5]

The registrant provided the requested sediment simulation test on the Substance on 14 February 2022. The eMSCA concluded its substance evaluation based on the results of the new study and all available information.

[3] Substance evaluation decision on UVASorb HEB: https://echa.europa.eu/documents/10162/d26ceb5d-6fdf-dd2f-da90-4f12aae1a596
[4] Decision of the BoA on UVASorb HEB (Case A-004-2017): https://echa.europa.eu/documents/10162/e1dbc57a-eeab-996f-2302-04ab737658ff
[5] Judgment of the General Court on UVASorb HEB (Case T-176/19): https://curia.europa.eu/juris/liste.jsf?language=en&td=ALL&num=T-176/19

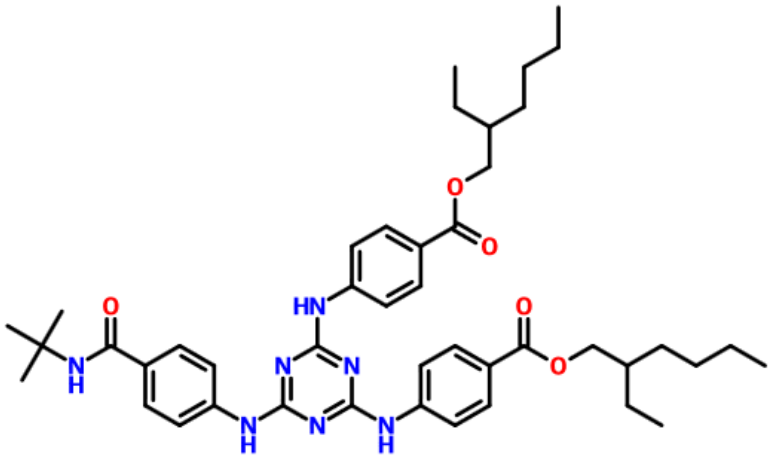
7.3. Identity of the substance

Table 4

SUBSTANCE IDENTITY	
Public name:	bis(2-ethylhexyl) 4,4'-{6-[4-tert-butylcarbamoyl) anilino]-1,3,5-triazine-2,4-diyldiimino} dibenzoate
EC number:	421-450-8
CAS number:	154702-15-5
Index number in Annex VI of the CLP Regulation:	-
Molecular formula:	$C_{44}H_{59}N_7O_5$
Molecular weight range:	765.99 g/mol
Synonyms:	▫ Diethylhexyl butamido triazone ▫ Dioctylbutamidotriazone ▫ Iscotrizinol ▫ UVASorb HEB

Type of substance: Mono-constituent

Structural formula:



7.4. Physico-chemical properties

Table 5

<table>
<tr><th colspan="2">OVERVIEW OF PHYSICOCHEMICAL PROPERTIES</th></tr>
<tr><th>Property</th><th>Value</th></tr>
<tr><td>Physical state at 20°C and 101.3 kPa</td><td>white, odourless powder</td></tr>
<tr><td>Melting point</td><td>88.3 – 91.4°C at 101.3 kPa
(Experimental result: EU Method A.1 (Melting / Freezing Temperature); capillary method)</td></tr>
<tr><td>Boiling point</td><td>>= 343.5 - <=351.6°C at 100.3 kPa
(Experimental result: OECD TG 103 (Boiling point), capillary method)</td></tr>
<tr><td>Vapour pressure</td><td>< 0.00019 Pa at 25°C
(Experimental result: OECD TG 104 (Vapour Pressure Curve), EU Method A.4 (Vapour Pressure); effusion method: vapour pressure balance)</td></tr>
<tr><td>Water solubility</td><td>< 0.00075 mg/L at 20.0±0.5°C, pH= 5.4 – 7.1
(Experimental result: EU Method A.6 (Water Solubility), OECD TG 105 (Water Solubility); column elution method)</td></tr>
<tr><td>Partition coefficient n-octanol/water (Log K_{ow})</td><td>log P_{ow} = 5.925 ± 0.100 (at 25°C) (experimental result: OECD TG 117 (Partition Coefficient (n-octanol / water), HPLC Method))

log P_{ow} = 4.12 ± 0.20 (at 20°C, pH 6.2) (experimental result: EU Method A.8 (Partition Coefficient (n-octanol / water), HPLC Method))
log P_{ow} = 14.03 (predicted result: KOWWIN[6])
log P_{ow} = 11.1009 (predicted result: COSMOtherm[7])
log P_{ow} = 12.392 (predicted result: chemicalize[8])</td></tr>
<tr><td>Granulometry</td><td><table><tr><th>Size</th><th>Distribution</th><th>Method</th></tr><tr><td>< 100 µm</td><td>97.3%</td><td>Sieve</td></tr><tr><td>< 10 µm</td><td>0.256%</td><td>Cascade Impactor</td></tr><tr><td>< 5.5 µm</td><td>0.204%</td><td>Cascade Impactor</td></tr></table>
(Experimental result: OECD TG 110 (Particle Size Distribution / Fibre Length and Diameter Distributions))</td></tr>
</table>

[6] KOWWIN v1.69; U.S. Environmental Protection Agency, 2015.

[7] COSMOconf conformer generation performed using the BP-SVP-AM1-COSMO+GAS template; COSMOtherm property estimation performed using the BP_SVP_AM1_21-parameterisation; BIOVIA COSMOtherm, Release 2021; Dassault Systèmes. http://www.3ds.com; BIOVIA COSMOconf, Release 2021; Dassault Systèmes. http://www.3ds.com

[8] Chemicalize, October 2022, https://chemicalize.com/ developed by ChemAxon (http://www.chemaxon.com).

7.5. Manufacture and uses

7.5.1. Quantities

Table 6

AGGREGATED TONNAGE (PER YEAR)				
☐ 1 – 10 t	☐ 10 – 100 t	x 100 – 1000 t	☐ 1000- 10,000 t	☐ 10,000-50,000 t
☐ 50,000 – 100,000 t	☐ 100,000 – 500,000 t	☐ 500,000 – 1000,000 t	☐ > 1000,000 t	☐ Confidential

7.5.2. Overview of uses

Table 7:

DESCRIPTION OF IDENTIFIED USES	
Life-cycle stage	**Use(s)**
Uses as intermediate	N/A
Formulation	Formulation into mixtures (UV filter for cosmetic products)
Uses at industrial sites	N/A
Uses by professional workers	N/A
Consumer Uses	Used as UV-Filter in cosmetics and personal care products (PC 39) for consumer uses in private households (SU 21).
Article service life	N/A

7.6. Classification and Labelling

7.6.1. Harmonised Classification (Annex VI of CLP)

The Substance does not have a harmonised classification.

7.6.2. Self-classification

The Substance is not classified in the registrations, except for one Registrant who self-classifies as Aquatic Chronic 4 H413.

The following hazard classes are in addition notified among the aggregated self-classifications in the C & L Inventory:

Aquatic Chronic 3 H412
Aquatic Chronic 4 H413

7.7. Environmental fate properties

7.7.1. Degradation

7.7.1.1. Hydrolysis

An aqueous hydrolysis pre-test (OECD TG 111) indicates that the Substance is hydrolytically stable (<10% hydrolysis). Combining the information of structural aspects (ester and amide bonds), it cannot be ruled out that the Substance does hydrolyse. Under environmental relevant conditions, the Substance is generally hydrolytically stable with a half-life likely >1 year.

7.7.1.2. Phototransformation/photolysis

No data available but typically the use of UV filters for cosmetic products suggests the stability of the substance under light exposure.

7.7.1.3. Biodegradation in water

Biodegradation of the Substance was tested in two screening tests and one simulation test.

Screening tests

There are two screening tests on biodegradation available. As stated by the registrants both key studies on biodegradation conform with GLP.

Table 8

SUMMARY OF SCREENING TESTS ON READY BIODEGRADABILITY			
Method	**Results**	**Remarks**	**Reference**
Test type: ready biodegradability activated sludge, domestic, adaptation not specified OECD Guideline 301B Ready Biodegradability (CO_2 Evolution Test)	not readily biodegradable. 8% degradation of the test substance after 28 d.	2 (reliable with restrictions)	ECHA 2022a
Test type: ready biodegradability activated sludge, domestic, adaptation not specified OECD Guideline 301B (Ready Biodegradability: CO_2 Evolution Test)	not readily biodegradable. 6% degradation of test substance after 28 d.	1 (reliable without restriction) key study experimental result	ECHA 2022a

In conclusion, the Substance is not readily biodegradable. The formation of transformation products of the Substance within these screening tests was not analytically determined.

Simulation tests

A valid simulation study on biodegradation in water and sediment according to OECD TG 308 is available. Radiolabelling was applied and to identify potential metabolites/transformation products the study was conducted at 20 °C. Samples of sediment and water were taken from a fluvial system near Milan and from the sea at the Ligurian Coast.

The mean total recovery was 101% for the fluvial system and 106% for the marine system. For both systems, no decline of the concentration of the Substance was observed, i.e., degradation of the substance was 0% after 102 days for the fluvial system and after 100 days for the marine system. Transformation products were not investigated since no degradation of the test substance higher than the 10% of the initial amount was observed.

Table 9

SUMMARY OF SIMULATION TESTS ON BIODEGRADATION IN WATER AND SEDIMENT			
Method	**Results**	**Remarks**	**Reference**
OECD Guideline 308 (Aerobic and Anaerobic Transformation in Aquatic Sediment Systems)	0% degradation observed after 100 d / 102 d.	1 (reliable without restriction)	ECHA 2022a

7.7.1.4. Biodegradation in soil

There are no data available.

7.7.1.5. Discussion of possible biodegradation pathways and persistent metabolites

There are estimations on the biotic degradation pathway of the Substance in the environment. To the knowledge of the eMSCA, no studies exist describing the biodegradation pathway of the Substance in the environment. Therefore, the eMSCA simulated the degradation pathways of the Substance with the EAWAG Biocatalysis/Biodegradation Prediction System.[9] This web application is a rule-based system currently compassing of 250 microbial biotransformation rules based on over 1350 microbial catabolic reactions and around 200 biodegradation pathways. The system compares the organic functional groups of the entered molecules with its set of rules and shows all possible degradation steps. The reaction steps are colour coded according to the likelihood that the respective reaction is catalysed by certain microorganisms in water, soil, or sediment. An overview of the system can be found in publications by Ellis et al. (Ellis et al., 2008, 2012) and Gao et al. (Gao et al., 2010, 2011). It is not possible to predict rate constants with this system. Also, there is no defined applicability domain for this rule-based system.

As the Substance is a complex molecule, the degradation pathway is also quite complex. In summary, with the eMSCA's current knowledge on the mechanism of the biodegradation

[9] http://eawag-bbd.ethz.ch/predict/ (accessed March 2023)

of 1,3,5-triazines, it seems reasonable to assume that they will be degraded slowly in the environment. Accordingly, among the total predicted transformation products (Figure 1), several metabolites containing the 1,3,5-triazine ring are identified as potentially P/vP as shown by BIOWIN 4.1 (Table 11). Many of these transformation products contain one or more carboxylic acid groups, which may ionize and dissociate under environmental relevant pH ranges. No registration- or CAS numbers were found for the corresponding SMILES of the likely formed metabolites except for 2,4,6-Triamino-*s*-triazin (see Table 10 below, compound 9).

Figure 1. EAWAG results for pathway prediction modelling of UVASorb HEB indicating the likelihood that transformation products will be formed (green: likely; yellow: neutral)

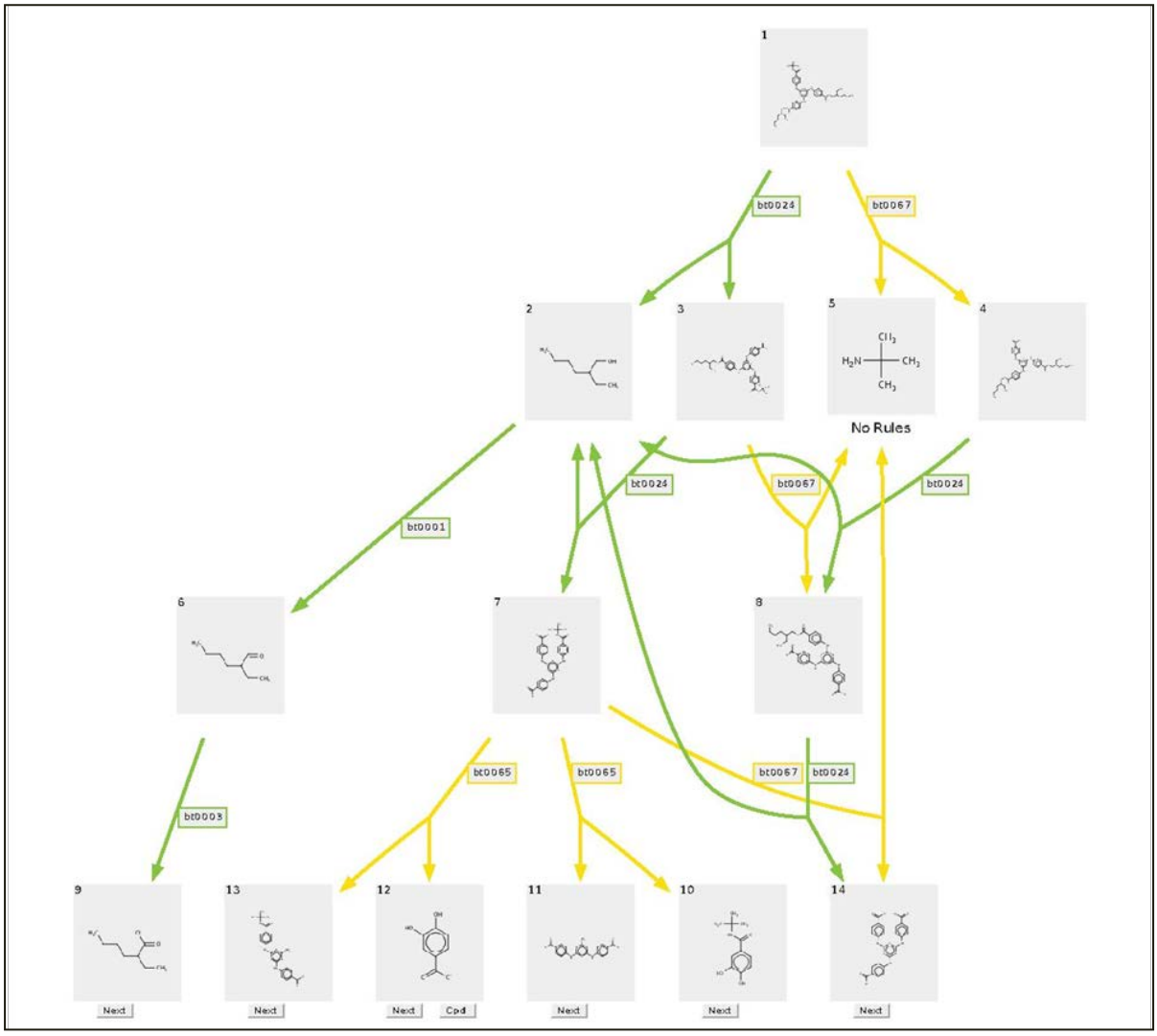
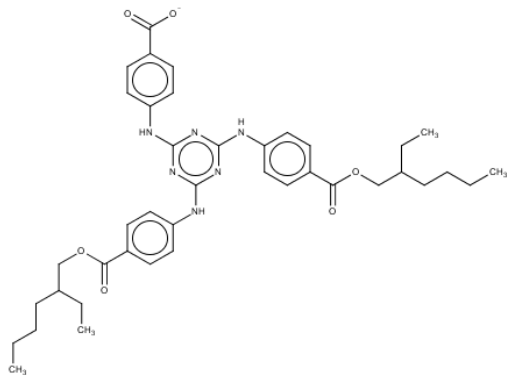
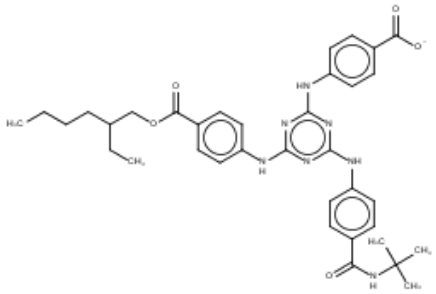
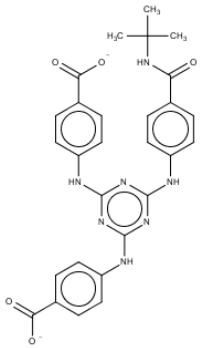
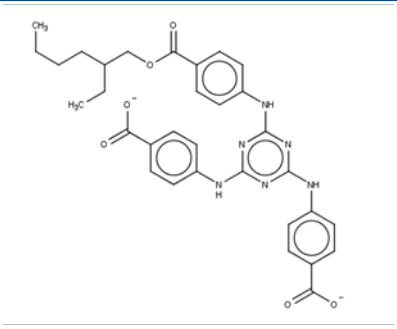
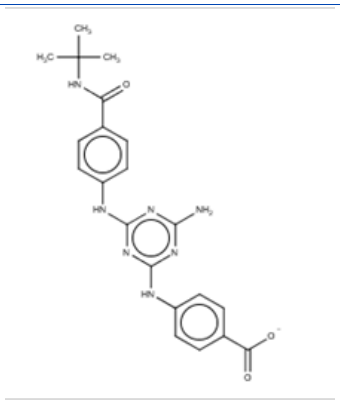
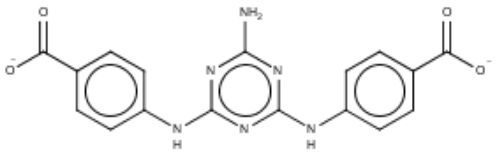
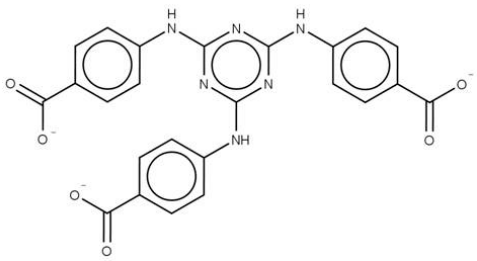
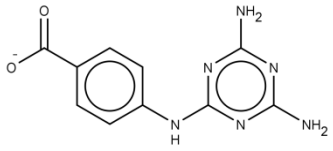
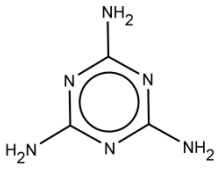


Table 10

OVERVIEW OF STRUCTURE AND QSAR ESTIMATIONS PROVIDED BY THE REGISTRANT(S) AND BASED ON OWN CALCULATIONS REGARDING P, B AND T SCREENING CRITERIA OF RELEVANT TRANSFORMATION PRODUCTS OF UVASORB HEB*		
Nr	**Structure and SMILES code**	**Physico-chemical and potential persistent properties***
1	 CCCCC(CC)COC(=O)c1ccc(Nc2nc(Nc3ccc(cc3)C([O-])=O)nc(Nc3ccc(cc3)C(=O)OCC(CC)CCCC)n2)cc1	Molecular weight = 710.88 g/mol Log K_{ow} = 13.33 (estimated) log K_{lipw}** = 8.90 L/kg Dissociated fraction (pH 7): 99.6% Hydrowin (pH 4/8): Half-life > 1 year Biowin2 (non-linear model): 0.0139 Biowin3 (ultimate deg. time): 1.942 Biowin6 (MITI-non-linear model): 0.0000 (Does not biodegrade fast/not readily biodegradable) **Conclusion on P: potentially P/vP** **T potentially fulfilled**
2	 CCCCC(CC)COC(=O) c1ccc (Nc2nc (Nc3ccc(cc3) C([O-]) =O) nc (Nc3ccc(cc3) C(=O) NC(C)(C) C) n2) cc1	Molecular weight = 653.79 g/mol Log K_{ow} = 10.31 (estimated) Hydrowin (pH 7/8): Half-life > 1 year Biowin2 (non-linear model): 0.0002 Biowin3 (ultimate deg. time): 1.3638 Biowin6 (MITI-non-linear model): 0.0000 (Does not biodegrade fast/not readily biodegradable) **Conclusion on P: potentially P/vP** **T potentially fulfilled**
3	 CC(C)(C) NC(=O) c1ccc (Nc2nc (Nc3ccc(cc3) C([O-]) =O) nc (Nc3ccc(cc3) C([O-]) =O) n2) cc1	Molecular weight = 541.57 g/mol Log K_{ow} = 6.60 (estimated) log K_{lipw} = 4.80 L/kg Dissociated fraction (pH 7): 99.0% Hydrowin (pH 4/8): Half-life > 1 year Biowin2 (non-linear model): 0.177 Biowin3 (ultimate deg. time): 1.26 Biowin6 (MITI-non-linear model): 0.0000 (Does not biodegrade fast/not readily biodegradable) **Conclusion on P: potentially P/vP** **T potentially fulfilled**

OVERVIEW OF STRUCTURE AND QSAR ESTIMATIONS PROVIDED BY THE REGISTRANT(S) AND BASED ON OWN CALCULATIONS REGARDING P, B AND T SCREENING CRITERIA OF RELEVANT TRANSFORMATION PRODUCTS OF UVASORB HEB*		
Nr	**Structure and SMILES code**	**Physico-chemical and potential persistent properties***
4	 CCCCC(CC)COC(=O) c1ccc (Nc2nc (Nc3ccc(cc3) C([O-]) =O) nc (Nc3ccc(cc3) C([O-]) =O) n2) cc1	Molecular weight = 598.66 g/mol Log K_{ow} = 9.62 (estimated) log K_{lipw} = 6.50 L/kg Dissociated fraction (pH 7): 99.2% Hydrowin (pH 7): Half-life > 1 year Biowin2 (non-linear model): 0.0021 Biowin3 (ultimate deg. time): 1.839 Biowin6 (MITI-non-linear model): 0.0000 (Does not biodegrade fast/not readily biodegradable) **Conclusion on P: potentially P/vP** **T potentially fulfilled**
5	 CC(C)(C)NC(=O)c1ccc(Nc2nc(N)nc(Nc3ccc(cc3)C([O-])=O)n2)cc1	Molecular weight = 421.46 g/mol Log K_{ow} = 4.50 (estimated) log K_{lipw} = 4.14 L/kg Dissociated fraction (pH 7): 88.72% Hydrowin (pH 7): Half-life > 1 year Biowin2 (non-linear model): 0.000 Biowin3 (ultimate deg. time): 1.438 Biowin6 (MITI-non-linear model): 0.0000 (Does not biodegrade fast/not readily biodegradable) **Conclusion on P: potentially P/vP** **T potentially fulfilled**
6	 Nc1nc (Nc2ccc(cc2) C([O-]) =O) nc (Nc2ccc(cc2) C([O-]) =O) n1	Molecular weight = 366.34 g/mol Log K_{ow} = 3.81 (estimated) log K_{lipw} = 3.64 L/kg Dissociated fraction (pH 7): 87.52% Hydrowin: cannot be estimated for this structure Biowin2 (non-linear model): 0.0002 Biowin3 (ultimate deg. time): 1.914 Biowin6 (MITI-non-linear model): 0.0000 (Does not biodegrade fast/not readily biodegradable) **Conclusion on P: potentially P/vP**
7		Molecular weight = 486.45 g/mol Log K_{ow} = 5.91 (estimated) log K_{lipw} = 4.11 L/kg Dissociated Fraction (pH 7): 99.2% Hydrowin: Half-life > 1 year Biowin2 (non-linear model): 0.0003 Biowin3 (ultimate deg. time): 1.7371

OVERVIEW OF STRUCTURE AND QSAR ESTIMATIONS PROVIDED BY THE REGISTRANT(S) AND BASED ON OWN CALCULATIONS REGARDING P, B AND T SCREENING CRITERIA OF RELEVANT TRANSFORMATION PRODUCTS OF UVASORB HEB*		
Nr	**Structure and SMILES code**	**Physico-chemical and potential persistent properties***
	[O-]C(=O)c1ccc(Nc2nc(Nc3ccc(cc3)C([O-])=O)nc(Nc3ccc(cc3)C([O-])=O)n2)cc1	Biowin6 (MITI-non-linear model): 0.0000 (Does not biodegrade fast/not readily biodegradable) **Conclusion on P: potentially P/vP** **T potentially fulfilled**
8	 Nc1nc(N)nc (Nc2ccc(cc2) C([O-]) =O) n1	Molecular weight = 246.23 g/mol Log K_{ow}= 1.71 (estimated) Hydrowin: cannot be estimated for this structure Biowin2 (non-linear model): 0.0001 Biowin3 (ultimate deg. time): 2.0922 Biowin6 (MITI-non-linear model): 0.0000 (Does not biodegrade fast/not readily biodegradable) **Conclusion on P: potentially P/vP**
9	 Nc1nc(N)nc(N)n1	Molecular weight = 126.12 g/mol Log K_{ow}= -0.38 (estimated) Log K_{ow}= -1.37 (experimental) Hydrowin: cannot be estimated for this structure Biowin2 (non-linear model): 0.0000 Biowin3 (ultimate deg. time): 2.2697 Biowin6 (MITI-non-linear model): 0.0000 (Does not biodegrade fast/not readily biodegradable) **Conclusion on P: potentially P/vP**

* Using COSMOmic 1504/ EAWAG Pathway Prediction System/EPISuite/ T.E.S.T./VEGA
**Membrane-Water-Partition-Coefficient (K_{Lipw})
Note: The documentation of the QSAR results does not comply with REACH Annex XI, hence their reliability is limited.

7.7.2. Summary and discussion on degradation

The Substance is not readily biodegradable as shown by screening tests. No degradation of the Substance was observed in a water sediment simulation test.

In summary, it is concluded that the Substance is very persistent.

While the formation of metabolites /transformation products is predicted by *in silico* tools, no metabolites/transformation products were observed in the available water sediment study.

7.7.3. Environmental distribution

7.7.3.1. Adsorption/desorption

Table 11

SUMMARY OF STUDIES ON ADSORPTION			
Method	**Results**	**Remarks**	**Reference**
Study type: adsorption/desorption screening test (soil) HPLC screening method OECD TG 121 method	Adsorption coefficient K_{oc}: 4.27 x 10^5 l/kg (Log K_{oc}: 5.63)	1 (reliable without restriction) key study experimental result	ECHA 2022a

Due to the high adsorption potential and the low water solubility, the available data support the conclusion that the Substance may be expected to distribute in soil and sediment and in lesser amounts in the water phase.

7.7.4. Bioaccumulation

7.7.4.1. Aquatic bioaccumulation

For the Substance, no experimental BMF or BCF study is available at present. However, other information can be used in a weight of evidence-approach:

Lipophilicity

The registration dossiers contain experimental *n*-octanol/water partition coefficient values (log K_{ow}) of 4.12 and 5.925 that were generated by the HPLC method. However, calculated values[10] strongly differ from the measured ones; KOWWIN[11], COSMOtherm[12] and Chemicalize[13] predict much higher log K_{ow} values of 14.03, 11.1009 and 12.392, respectively. Furthermore, an experimental log K_{ow} > 7 is available for the structurally related substance Uvinul T150 (CAS 88122-99-0, EC 402-070-1, see Table 12).

While it should be noted that the Substance exceeds the fragment instance domain and the molecular weight range of the KOWWIN training set, KOWWIN was shown to yield good results for the subset of the validation set that was both outside molecular weight range and the fragment instance domain.[14] The Substance was inside the molecular weight range of the respective validation set. The application domain of Chemicalize is not known. COSMOtherm is based on the COSMO-RS theory (Klamt 2011) and is not calibrated to

[10] SMILES code used:
CCCCC(CC)COC(=O) C1=CC=C(NC2=NC(NC3=CC=C(C=C3) C(=O) OCC(CC)CCCC) =NC(NC3=CC=C(C=C3) C(=O) NC(C)(C) C) =N2) C=C1
[11] KOWWIN v1.69; U.S. Environmental Protection Agency, 2015.
[12] COSMOconf conformer generation performed using the BP-SVP-AM1-COSMO+GAS template; COSMOtherm property estimation performed using the BP_SVP_AM1_21-parameterisation;
BIOVIA COSMOtherm, Release 2021; Dassault Systèmes. http://www.3ds.com;
BIOVIA COSMOconf, Release 2021; Dassault Systèmes. http://www.3ds.com
[13] Chemicalize, October 2022, https://chemicalize.com/ developed by ChemAxon (http://www.chemaxon.com).
[14] KOWWIN v1.69; U.S. Environmental Protection Agency, 2015.

experimental log K_{ow} data. Therefore, there is no applicability domain, and it is applicable to a broader range of substances than KOWWIN and Chemicalize.

Based on the molecular structure, the very low water solubility of < 0.00075 mg/L and the high molecular weight, the Substance is expected to be highly lipophilic. Substances with such high lipophilicity are outside the applicability domain of the HPLC method. Hence, the experimental values might be artefacts.

QSAR methods like KOWWIN are generally considered of similar quality like HPLC data; in case of log K_{ow} values > 6 it is considered that QSAR data are preferable. Based on the available data, it is concluded that UVASorb HEB has a log K_{ow} value > 7, potentially > 10. Due to this high lipophilicity, bioaccumulation testing may be technically challenging and susceptible to artefacts.

Read-across to Uvinul T150 shown to be <u>not</u> B or vB

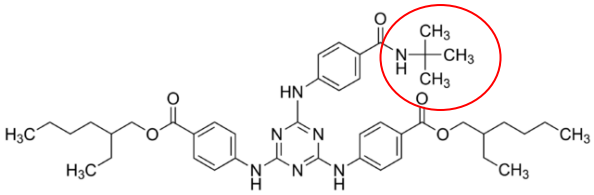
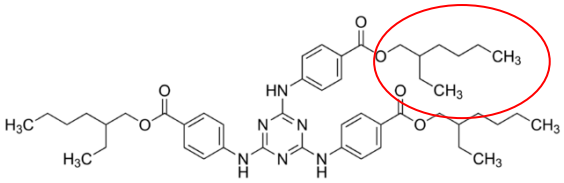
A read-across from the structurally very closely related substance Uvinul T150 (CAS 88122-99-0, EC 402-070-1, cf. Table 12) to the Substance indicates that it might not be B or vB. A BCF flow through test with Uvinul T150 according to OECD 305 revealed a mean kinetic BCF of 77 L/kg wet-wt with measured test concentrations in the flow-through system of 0.02 and 0.10 µg/L (BAuA 2016). The test was conducted with ^{14}C-labeled Uvinul T150 in zebrafish (*Danio rerio*) over an uptake period of 28 days followed by a depuration period of 16 days. Test concentrations were kept constant within the range of +20% of the nominal concentration with some exceptions. During the exposure to the test substance no toxic effects like mortality or changes in behavior or appearance were observed in the test organisms. This study was also reviewed by RAC during a CLH consultation; RAC concluded that UVINUL T150 has a low potential for bioaccumulation (RAC 2016).

<u>Rationale for read-across assessment</u>

According to the legal text of REACH, particularly Annex XI, 1.5 and the 'Read-across assessment framework (RAAF)' published by ECHA, the aim of a read-across is to avoid testing of every substance for every endpoint by using data known for one substance – in this case of the environmental fate - for other, similar substances. Substance similarity may be based on three criteria:
(i) a common functional group.
(ii) common precursors and/or the likelihood of common breakdown products via physical and biological processes, which result in structurally similar chemicals; or
(iii) a constant pattern in the changing of the potency of the properties.

All three points are met in this example: the two substances differ only in one functional group (Table 12), and they have similar physico-chemical properties. Moreover, pathway prediction models show that both compounds degrade to partly the same breakdown products. Additionally, the two substances are expected to have very similar environmental behaviour. No data are available on the formation and bioaccumulative properties of relevant metabolites of Uvinul T150.

Table 12

MOLECULAR STRUCTURE, PHYSICO-CHEMICAL PROPERTIES AND OTHER PARAMETERS	
UVASorb HEB	**Uvinul T150**
	
Differing functional group: 1-amino-2,2-dimethyl-ethane bonded via an **amide** group to the main molecule Log K_{ow} : 4.12; 5.925; 11.1009; 12.392; 14.03 (EC A.8, HPLC, COSMOtherm, Chemicalize, KOWWIN) Log K_{oc}: 5.63 (OECD 121) Molecular weight=765.99 g/mol	Differing functional group: 2-ethyl-hexanol bonded via an **ester** group to the main molecule Log K_{ow}: >7 at 20 °C (EC A.8) Log K_{oc}: 5.63 (OECD Guideline 121) Molecular weight= 823.10 g/mol

Repeated dose toxicity data with rats:

A repeated dose toxicity data in rats according to OECD TG 408 (Repeated oral Toxicity in Rodents dietary study) show complete absence of effects of the Substance in the long term, indicating that either the parent substance is not toxic or that is not taken up to a significant extent by mammals. A Combined Reproduction/Developmental Toxicity Screening study with rats according to OECD TG 421 (oral gavage) showed clinical signs in the high-dose group (1000 mg/kg bw/d) which can be attributed to the test compound (NOAEL at 500 mg/kg bw/d). Therefore, some gastro-enteric absorption as well as systemic distribution must be assumed at the high dose of 1000 mg/kg bw/d.

Similar results were found for Uvinul T150: no effects were seen in an OECD TG 408 or OECD TG 414 (prenatal developmental toxicity study). However, it must be kept in mind that the results are not transferable to aquatic organisms.

Data on uptake in sediment organisms:

In a recent study, the ragworm *Hediste diversicolor* was exposed to the Substance via artificial spiked sediment (Clergeaud 2022). After 28 days of exposure, a BSAF (biota-sediment accumulation factor) of 0.3 was observed. This study shows that the Substance in sediment is taken up by sediment organisms. Many marine animals feed on the ragworm *Hediste diversicolor* and may thus be exposed to the Substance via the diet.

7.7.4.2. Terrestrial bioaccumulation

7.7.4.2.1. Screening data

A substance is considered as potentially bioaccumulating in airbreathing organisms if its log K_{OW} > 2 and its log K_{oa} > 5.

Both experimental and estimated log K_{OW} values are available, and all values are > 2. The octanol-air partition coefficient was estimated by KOAWIN[15]; predicted log K_{AW} values are > 5 (see Table 13). Hence, the screening criterion for terrestrial bioaccumulation is met.

Table 13

ESTIMATED OCTANOL-AIR PARTITION	
log K_{OW} used for prediction	**Predicted log K_{OA}**
exp log K_{OW} of 4.12	24.34
exp log K_{OW} of 5.925	26.15
pred log K_{OW} of 11.1009[16]	31.32
pred log K_{OW} of 12.392[17]	32.61
pred log K_{OW} of 14.03[18]	34.25

KOAWIN results for log K_{OA}. Calculations were conducted using both manually entered experimental log K_{OW} and predicted log K_{OW}.

7.7.4.2.2. Mammalian data

The repeated dose toxicity data with rats according to OECD TG 408 (Repeated oral Toxicity in Rodents dietary study) show complete absence of effects in the long term at concentrations up to 831 mg/kg bw/d (males) or 963 mg/kg bw/d (females), indicating that either the parent substance is not toxic or that is not taken up to a significant extent by mammals.

A Combined Reproduction/Developmental Toxicity Screening study with rats according to OECD TG 421 (oral gavage) showed clinical signs in the high-dose group (1000 mg/kg bw/d) which can be attributed to the test compound (NOAEL at 500 mg/kg bw/d). Therefore, some gastro-enteric absorption as well as systemic distribution must be assumed at the high dose of 1000 mg/kg bw/d.

7.7.4.2.3. Summary on terrestrial bioaccumulation

While the Substance fulfills the screening criteria for terrestrial bioaccumulation, there is no indication of bioaccumulation from the available mammalian data.

There is still no guidance for the testing or assessment of terrestrial bioaccumulation and hence, there is currently no adequate testing strategy to examine this property further.

[15] KOAWIN v1.11; U.S. Environmental Protection Agency, 2015.
[16] COSMOconf conformer generation performed using the BP-SVP-AM1-COSMO+GAS template; COSMOtherm property estimation performed using the BP_SVP_AM1_21-parameterisation;
BIOVIA COSMOtherm, Release 2021; Dassault Systèmes. http://www.3ds.com;
BIOVIA COSMOconf, Release 2021; Dassault Systèmes. http://www.3ds.com
[17] Chemicalize, October 2022, https://chemicalize.com/ developed by ChemAxon (http://www.chemaxon.com).
[18] KOWWIN v1.69; U.S. Environmental Protection Agency, 2015.

7.7.4.3. Summary and discussion on bioaccumulation data

The Substance has a log K_{ow} value >7, potentially >10 and thus fulfils the B/vB screening criterion. As the substance is highly hydrophobic, a very slow uptake and clearance kinetic can be expected and reaching the steady state concentration can last years (Larisch and Goss, 2018). Consequently, there is some concern for slow bioaccumulation. However, this is not covered by the current guidance and is therefore a development issue where more research is needed.

No bioaccumulation was observed in a fish bioaccumulation study on a structurally related substance. A recent study with ragworms showed that the substance can be taken up by sediment organisms. A Combined Reproduction/Developmental Toxicity Screening study with rats according to OECD TG 421 (oral gavage) indicated some potential for gastro-enteric adsorption and systemic distribution, at least when administered via oral gavage. In contrast, in a repeated-dose toxicity study (OECD TG 408) in rats in which the test compound was added to the diet in a comparable dose, there was no indication for absorption (no effects were observed).

While the Substance fulfills the screening criteria for terrestrial bioaccumulation, there is no indication of bioaccumulation from the available mammalian data.

Based on the current guidance (ECHA 2017) and the available data, the eMSCA concludes that it is unlikely that UVASorb HEB is bioaccumulative in organisms.

7.8. Environmental hazard assessment

7.8.1. Aquatic compartment (including sediment)

7.8.1.1. Fish

A short-term toxicity study on fish (*Danio rerio*) was conducted according to OECD TG 203 (Unpublished, 1997, Registration dossier). No effects were observed up to the range of the water solubility level of 0.0007 mg/L at nominal concentration of the substance of 10 mg/L (nominal) and 2.48 mg/L (measured). A solubiliser was applied to reach appropriate concentration of the Substance in the system. The LC_{50} (96 h) was >2.48 mg/L. The absence of toxic effects could basically be attributed to the reduced bioavailability of the Substance due to its extremely poor water solubility or to adsorption effects on vessel surfaces.

No long-term toxicity test on fish is available.

7.8.1.2. Aquatic invertebrates

A 48-h acute toxicity test with *Daphnia magna* was conducted in 1997 according to OECD TG 202 with a nominal concentration of the Substance of 10 mg/L and a measured concentration of 1.88 mg/L. A solubiliser was applied to reach appropriate concentration of the substance in the system. The EC_{50} (48 h) was > 1.88 mg/L. Hence, no acute toxic effects were observed up to the water solubility level of 0.00075 mg/L.

No long-term toxicity test to aquatic invertebrates is available.

7.8.1.3. Algae and aquatic plants

A 68-h toxicity test on green algae (*Pseudokirchneriella subcapitata*) was conducted according to OECD TG 201 (Unpublished, 1997, Registration dossier). No effects were observed within the range of the solubility at nominal concentrations of 10 mg/L. A solubiliser was applied to reach the appropriate concentration of the substance in the system. The NOEC (growth) and (biomass) was 2.7 mg/L. This indicates that the Substance is not acute or chronic toxic to algae.

7.8.1.4. Sediment organisms

No data available.

7.8.1.5. Other aquatic organisms

No data available.

7.8.1.6. Estimated Data

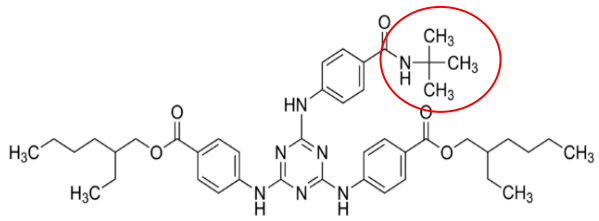
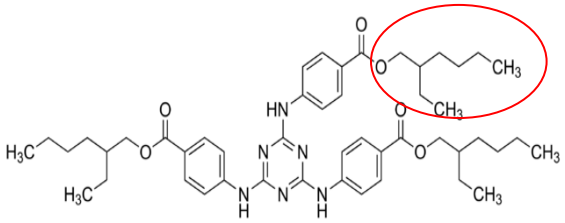
QSAR predictions regarding toxicity of the parent compound

The registrants provided QSAR modelling for the estimation of chronic toxicity to algae, daphnia, and fish by applying ECOSAR, T.E.S.T. and VEGA. Actual measured log K_{ow} (4.12) and water solubility (0.00075 mg/L) values were introduced into the model. The results from the modelling are consistent with short-term tests indicating no toxic effects to algae, daphnia, or fish. However, some estimates were outside applicability domain of the model.

Read-across from Uvinul T150 to the Substance

As already pointed out under 7.7.4, a read-across from Uvinul T150 to the Substance is considered as adequate. A long-term toxicity study of Uvinul T150 with fish according to OECD 210 revealed a NOEC (35 d) of >1.01 µg/L. A long-term toxicity test with invertebrates (*Daphnia magna*) according to OECD 211 revealed a NOEC (21 d) > 1 µg/L. The analytical results of the tests indicate that the tested concentrations were still above the water solubility limit of the test substance (< 1 µg/L at 20°C, Unpublished, 2008b, registration dossier). Provided that the Substance has similar toxic effects as Uvinul T150 due to structural similarities and similar physico-chemical properties (Table 13), it is unlikely that the Substance fulfils the T-screening criterion as stated under REACH, Annex XIII.

Table 14

MOLECULAR STRUCTURE, PHYSICO-CHEMICAL PROPERTIES AND OTHER PARAMETERS OF UVASORB HEB AND UVINUL T150	
UVASorb HEB	**Uvinul T150**
	
Differing functional group: - 1-amino-2,2-dimethyl-ethane bonded via an **amide** group to the main molecule Available data on toxicity: ➔ No acute effects (OECD TG 201/202/203) ➔ QSAR estimated chronic toxicity (daphnia/fish): no effects predicted ➔ Not toxic to mammals (OECD TG 408/421)	Differing functional group: - 2-ethyl-hexanol bonded via an **ester** group to the main molecule Available data on toxicity: ➔ No acute effects (OECD TG 201/202/203) ➔ No chronic effects on algae/daphnia/fish ➔ Not toxic to mammals (OECD TG 408/414)

7.8.2. Terrestrial compartment

No data available.

7.8.3. Toxicity studies with mammals

Repeated dose toxicity data in rats according to OECD TG 408 (Repeated oral Toxicity in Rodents dietary study) did not show any effects.

In a Combined Reproduction/Developmental Toxicity Screening study in rats according to OECD TG 421, administration of Uvasorb ® HEB by oral gavage resulted in clinical signs in the highest dose group of 1000 mg/kg bw/d, including for example reduced grooming, signs of respiratory distress, hunched posture, and white, red and/or brown perioral substance. One male and one female of the highest dose group were euthanised due to adverse clinical signs. Moreover, in the highest tested dose group of 1000 mg/kg bw/d, reduced body weight gain (–22% over the entire dosage period in males; –65% from premating dosing day 1 to 14) as well as reduced food consumption from dosing days 1 to 14 only in males (–7%) were observed. There were no effects on fertility and no clinical signs were observed in the offspring.

7.8.4. Microbiological activity in sewage treatment systems

A study according to OECD TG 209 with activated sludge was conducted (Unpublished, 2008, Registration dossier) and showed no toxic effects of UVASorb HEB to microorganisms (EC_{50} (3 h) > 1 mg/L).

7.8.5. Conclusions for classification and labelling

Based on the available information, the eMSCA considers that the Substance does not fulfil the criteria for aquatic toxicity according to CLP. It is also not self-classified for mammalian toxicity.

7.8.6. Summary and discussion on toxicity data

Several data assessed in a weight of evidence approach provide evidence that the Substance does not screen as toxic to aquatic organisms.

7.9. Human Health hazard assessment

Not assessed.

7.10. Assessment of endocrine disrupting (ED) properties

Not assessed.

7.11. PBT and vPvB assessment

7.11.1. Persistence

The Substance is not readily biodegradable as shown by screening tests. No degradation of UVASorb HEB was observed in a water sediment simulation test. In summary, it is concluded that the Substance is very persistent.

While the formation of metabolites /transformation products is predicted by *in silico* tools, no metabolites/transformation products were observed in the available water sediment study.

7.11.2. Bioaccumulation

The available data on bioaccumulation includes predicted and measured Log K_{ow} values, read-across to a structurally related substance and data for sediment organisms and toxicokinetic data. Currently, these data do not indicate that the Substance is bioaccumulative in aquatic organisms.

While the Substance fulfills the screening criteria for terrestrial bioaccumulation, there is no indication of toxicity or bioaccumulation from the available mammalian data.

The high hydrophobicity of the Substance raises a concern for slow bioaccumulation which however cannot be investigated further with existing validated methods.

7.11.3. Toxicity

Several data assessed in a weight of evidence approach provide evidence that the Substance does not screen as toxic to aquatic organisms or mammals.

7.11.4. Overall conclusion of PBT / vPvB assessment

Based on the available data, the Substance does not fulfil the PBT/vPvB criteria of REACH Annex XIII.

7.12. Exposure assessment

The exposure assessment was targeted on the environment.

The Substance is used as a UV-filter in personal care products and is expected to enter the environment via wastewater, direct discharges or directly into swimming waters. Due to the high adsorption potential (log K_{oc} = 5.63), the main portion of the Substance will adsorb on sediment and on sewage sludge of municipal wastewater treatment plants, which might be applied on agricultural soils, thereafter, increasing the likelihood that terrestrial organisms will also be exposed. Consequently, all compartments, except air, may be exposed to the Substance. Due to insufficient information regarding environmental release estimation, it is not possible to conclude on possible risks for the environment from manufacture, formulation, and uses of the Substance. This concerns the selected emission factors.

It must be noted that the registration documents do not contain an exposure assessment. The Substance is currently not (self)-classified as hazardous under the CLP regulation. Therefore, an exposure assessment and an environmental risk characterisation are currently not required under REACH. Previously reported exposure assessments might not be valid anymore.

7.13. Risk characterisation

Not assessed.

7.14. References

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Gao J, Ellis LBM, Wackett LP 2010 "The University of Minnesota Biocatalysis/Biodegradation Database: improving public access" Nucleic Acids Research 38: D488-D491.

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RAC 2016. Committee for Risk Assessment. Opinion proposing harmonised classification and labelling at EU level of tris(2-ethylhexyl) 4,4',4''-(1,3,5-triazine-2,4,6-triyltriimino) tribenzoate. EC Number: 402-070-1, CAS Number: 88122-99-0, CLH-O-0000001412-86-129/F, https://echa.europa.eu/documents/10162/70720828-d593-2bc8-e432-6044c67999b3 (accessed July 2022)

7.15. Abbreviations

B	bioaccumulative (pertaining to Annex XIII REACH)
BAF	bioaccumulation factor
BCF	bioconcentration factor
BMF	biomagnification factor
BMF_K	growth corrected kinetic biomagnification factor
BSAF	biota-sediment accumulation factor
CAS RN	CAS registry number
CLH	Harmonised classification and labelling
CLP	Classification, labelling, and packaging of substances
DT_{50}	degradation half-life
EC	effect concentration
eMSCA	evaluating Member State competent authority
GLP	Good Laboratory Practice
HPLC	high performance liquid chromatography
K_{OA}	octanol-air partition coefficient
K_{OC}	adsorption coefficient
K_{OW}	octanol-water partition coefficient
LC_{50}	Lethal concentration to 50% of test animals
MSC	Member State Committee
NOEC	no observed effect concentration
P	Persistent (pertaining to Annex XIII REACH)
PBT	persistent, bioaccumulative and toxic
PNEC	Predicted No Effect Concentration
QSAR	quantitative structure-activity relationship
RAAF	Read-across assessment framework
RAC	Committee for Risk Assessment
SEV	Substance Evaluation
SVHC	Substance of very high concern
T	Toxic (pertaining to Annex XIII REACH)
TG	Testing guideline
UM-PPS	University of Minnesota Biocatalysis/Biodegradation Prediction System
UVASorb HEB	bis(2-ethylhexyl) 4,4'-{6-[4-tert-butylcarbamoyl) anilino]-1,3,5-triazine-2,4-diyldiimino} dibenzoate
wet-wt	wet weight
vB	very bioaccumulative (pertaining to Annex XIII REACH)
vP	very persistent (pertaining to Annex XIII REACH)
vPvB	very persistent and very bioaccumulative (pertaining to Annex XIII REACH)