Annex XV dossier

PROPOSAL FOR IDENTIFICATION OF A SUBSTANCE AS A CMR 1A OR 1B, PBT, vPvB OR A SUBSTANCE OF AN EQUIVALENT LEVEL OF CONCERN

Substance Name(s): **2-benzotriazol-2-yl-4,6-di-tert-butylphenol (UV-320)**

EC Number(s): **223-346-6**

CAS Number(s): **3846-71-7**

Submitted by: **Germany**

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Substance Name(s): 2-benzotriazol-2-yl-4,6-di-tert-butylphenol

EC Number(s): 223-346-6

CAS number(s): 3846-71-7

- It is proposed to identify the substance(s) as PBT according to Article 57 (d).
- It is proposed to identify the substance(s) as vPvB according to Article 57 (e).

Summary of how the substance(s) meet(s) the criteria set out in Articles 57(d) and 57(e) of REACH

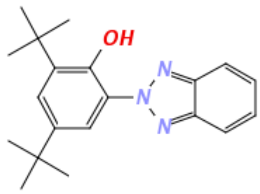
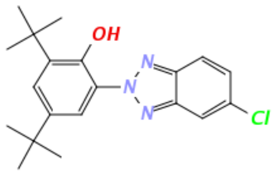
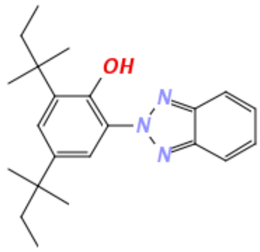
According to a Weight-of-Evidence argumentation UV-320 has to be considered vP and therefore also P. Also the substance fulfils in a MITI-study the numerical criterion to be considered vB and therefore also B. Finally, UV-320 fulfils also the criteria to be classified as STOT-RE 1 and therefore has to be considered as toxic. In conclusion UV-320 has vPvB- and PBT-properties.

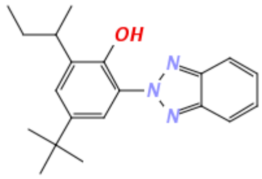
Registration dossiers available: No

PART I

Note: This dossier is one of four dossiers for the SVHC-identification of several phenolic benzotriazoles as vPvB-substances and in two cases also as PBT-substances. Since these substances are structurally very similar and relevant data on individual substances for some endpoints is scarce, in these instances all information for all four substances of the set is given to allow an assessment based on Read-Across and a Weight-of-Evidence-approach in an Analogue Approach. All relevant available experimental data on the substances in question is presented in a Read-Across-Matrix in Annex 1. In the individual chapters only the relevant data for assessing the individual endpoint will be presented. Parts that are identical in all documents will be from now on highlighted in green. Consequently, these chapters are identical in the four dossiers. The set of the four phenolic benzotriazoles composes of:

Table 1: Overview of the phenolic **benzotriazoles proposed for SVHC-identification**

Name	EC-nr.	CAS-nr.	Trade name used in this dossier	Structure
2-benzotriazol-2-yl-4,6-di-tert-butylphenol	223-346-6	3846-71-7	UV-320	
2,4-di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol	223-383-8	3864-99-1	UV-327	
2-(2H-benzotriazol-2-yl)-4,6-ditertpentylphenol	247-384-8	25973-55-1	UV-328	

2-(2H-benzotriazol-2-yl)-4-(tert-butyl)-6-(sec-butyl)phenol	253-037-1	36437-37-3	UV-350	

JUSTIFICATION

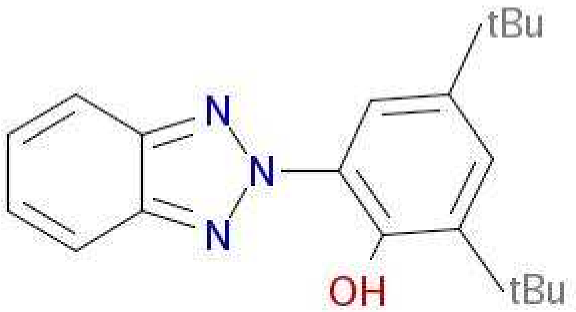
1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

Table 2: Substance identity

EC number:	223-346-6
EC name:	2-Benzotriazol-2-yl-4,6-di-tert-butylphenol
CAS number (in the EC inventory):	3846-71-7
CAS number:	3846-71-7
CAS name:	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-
IUPAC name:	2-(2H-benzotriazol-2-yl)-4,6-di-tert-butylphenol
Index number in Annex VI of the CLP Regulation	-
Molecular formula:	C20H25N3O
Molecular weight range:	323.432 g/mol
Synonyms:	2-(2'-Hydroxy-3',5'-di-t-butylphenyl)benzotriazole 2-(2'-Hydroxy-3',5'-di-tert-butylphenyl)benzotriazole 2-(2'-Hydroxy-3'5-di-tert-butylphenyl) benzotriazole 2-(2-Benzotriazolyl)-4,6-di-tert-butylphenol 2-(2-Hydroxy-3,5-di-tert-butylphenyl)-2H-benzotriazole 2-(2-Hydroxy-3,5-di-tert-butylphenyl)benzotriazole 2-(3',5'-Di-tert-butyl-2'-hydroxyphenyl)benzotriazole 2-(3,5-Di-tert-butyl-2-hydroxyphenyl)-2H-benzotriazole 2-(3,5-Di-tert-butyl-2-hydroxyphenyl)benzotriazole 2-Benzotriazol-2-yl-4,6-di-tert-butylphenol Benzotriazol-2-yl-4,6-di-tert-butyl-phenol

Structural formula:



1.2 Composition of the substance

Name: 2-benzotriazol-2-yl-4,6-di-tert-butylphenol

Description: mono-constituent substance

Degree of purity: ≥98 %[1]

Table 3: Constituents

As this substance is a monoconstituent substance this information in not relevant.

Constituents	Typical concentration	Concentration range	Remarks
2-benzotriazol-2-yl-4,6-di-tert-butylphenol EC Number: 223-346-6	≥98 %	≥98 % - 100 %	

Table 4: Impurities

Impurities	Typical concentration	Concentration range	Remarks
n.a.			

[1] From C&L notifications

Table 5: Additives

Additives	**Typical concentration**	**Concentration range**	**Remarks**
n.a.			

1.3 Physico-chemical properties

Table 6: Overview **of physicochemical properties**

Property	**Value**	**Remarks**
Physical state at 20°C and 101.3 kPa	-	-
Melting/freezing point	191 °C	result from MPBPWIN-module in EPISUITE v4.10; US EPA 2011
Boiling point	444.0 ± 55.0°C	calculated properties using Advanced Chemistry Development (ACD/Labs) Software V11.02 (©1994-2010 ACD/Labs)
Vapour pressure	$1.70*10^{-8}$ Torr, 25 °C	calculated properties using Advanced Chemistry Development (ACD/Labs) Software V11.02 (©1994-2010 ACD/Labs)
Water solubility	0.1503 mg/l at 25°C	QSAR estimation from log Kow with the EPISuite module WSkowWIN v1.42; US EPA 2011, log Kow used for calculation: 6.27
Partition coefficient n-octanol/water (log value)	6.853 ± 1.254, Temperature = 25 °C 6.27 7.39	calculated properties using Advanced Chemistry Development (ACD/Labs) Software V11.02 (©1994-2010 ACD/Labs) EPISuite v.4.10 COSMOtherm v. C30_1201
Dissociation constant	-	-
[enter other property, if relevant, or delete row]	-	-

2 HARMONISED CLASSIFICATION AND LABELLING

No harmonized or agreed classification is available for the substance. The self classifications according to Regulation 1272/2008/EC (CLP) from ECHA's C&L Inventory database are provided in Annex 2 to give some indications on the hazards of the substance.

3 ENVIRONMENTAL FATE PROPERTIES

3.1 Degradation

3.1.1 Abiotic degradation

3.1.1.1 Hydrolysis

The chemical bond between the benzotriazole group and the aromatic ring is generally expected to be very strong and also able to withstand degradation due to hydrolysis (see also 3.1.2.1.1) and also the aliphatic groups in the side chains of the phenol ring are functional groups that are expected to be generally resistant to hydrolysis. Due to the high log K_{OW} and the high adsorption potential to organic carbon the substance will adsorb to sewage sludge and suspended organic matter when it is released to the sewage treatment system, respectively to the aquatic environment.

Therefore hydrolysis is not expected to be a relevant pathway of removal of UV-320.

3.1.1.2 Phototransformation/photolysis

Phenolic benzotriazoles are mainly used as an UV-absorber. This means that on the molecular level UV-radiation excites the phenolic benzotriazole. In this excited state a proton from the OH-group is transferred to a nitrogen atom. From this structure a radiationless deactivation coupled with another proton transfer from the nitrogen back to the OH-group will bring the molecule back into its ground state. The UV-protection properties are based on this fully reversible and non-destructive process. Therefore degradation through photolysis can be regarded as a negligible degradation path, nevertheless the different compartments will be briefly discussed.

3.1.1.2.1 Phototransformation in air

An estimation for half-life in air due to degradation with OH-radicals has been conducted with AOPwin v1.91 (US EPA, 2011) assuming a 12 hour-day and a OH-concentration of $1.5*10^6$ OH-radicals/cm³.

The atmospheric half-life was estimated to be 9.534 hours, the overall OH-rate constant was estimated to be $1.346*10^{-11}$ cm³*molec^{-1}*sec^{-1}.

It is expected that photolytic degradation in air is no relevant pathway for removal from the environment. As it is assumed that the majority of UV-320 will be emitted indirectly via sewage treatment systems and directly via surface runoff into the aquatic compartment and considering the very low vapour pressure of UV-320 we conclude that the substance will not evaporate at ambient temperature. This assumption is supported by the results of environmental distribution modelling (please see section 3.3.2). Therefore photolytic degradation in the atmosphere is not considered to be relevant for the PBT assessment in the light of the partition properties of the substance.

3.1.1.2.2 Phototransformation in water

Photolytic degradation of UV-320 is expected to be a relevant degradation process only in very shallow clear waters and in the first few centimetres of the water column, decreasing rapidly in the lower layers of the water column, if at all. It is expected that the environmental exposure of the substance occurs in the whole water column. Because of the substance's adsorption potential it will predominantly bind to suspended organic matter and sediment which is supposed to decrease the tendency for photolytic degradation. Therefore aquatic photolytic degradation is not considered to have relevant impact on the overall persistency of UV-320 in the aquatic environment.

3.1.1.2.3 Phototransformation in soil

Information from industry indicates that a small fraction of the group of phenolic benzotriazoles is used in the EU in cosmetic products. The majority of this fraction will end up in waste water and finally adsorb at sewage sludge. As the use of this sludge is a common practice in agricultural industry soil will be subject to indirect exposure. As final step the sludge will be ploughed in and therefore only negligible quantities will be available for photolytic degradation processes.

This leads to the conclusion that photolysis is not a relevant pathway for removal of UV-320 in soil.

3.1.2 Biodegradation

3.1.2.1 Biodegradation in water

3.1.2.1.1 Estimated data

To our knowledge no studies exist describing the biodegradation pathway of the phenolic benzotriazoles in the environment. Therefore we simulated the pathways of all phenolic benzotriazoles in question together with the University of Minnesota Biocatalysis/Biodegradation Prediction System (UM-PPS[2]). This web application is a rule-based system currently compassing of 250 microbial biotransformation rules based on over 1350 microbial catabolic reactions and about 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 color coded according to the likelihood that the respective reaction is catalysed by certain bacteria in water, soil or sediment. An overview of the system can be found in two recent publications by Ellis et al. (Ellis et al., 2008) and Gao et al (Gao et al., 2011). Please not that it is not possible to predict rate constants with this system.

As the phenolic benzotriazoles are complex molecules their degradation pathway is also quite complex. Nevertheless a comparison of the results shows similarities and patterns. All the relevant reaction pathways for degradation of the bond between the phenol ring and the benzotriazole moiety begin with the stepwise degradation of the side chains in position four and six (the ortho and para-position to the hydroxyl group on the phenolic ring). The bond between the benzotriazole moiety and the phenolic ring is never directly cleaved. The UM-PPS predicts that the actual breakdown of the phenolic benzotriazole moiety begins only when two vicinal hydroxyl groups on the phenolic

[2] http://umbbd.msi.umn.edu/predict/ (accessed 12.06.2012)

ring are formed. In order to form the vicinal hydroxyl groups it is necessary to degrade the side chain in position six (ortho-position) first. Depending on the phenolic benzotriazole in question this encompasses many reaction steps that sometimes are not very likely (and therefore kinetically speaking slow). Of special importance in this regard is the reaction of the aliphatic methyl groups into primary alcohols. The crucial step after degradation of the side chain is reached when the two vicinal hydroxyl groups are formed. Now the carbon-carbon-bond between them is then broken and therefore the phenolic ring cleaved. The mechanism is shown in Figure 1. Please note that it is also possible that the benzene ring of the benzotriazole moiety is attacked, but this does not lead to the cleavage of the bond between the phenolic ring and the former benzotriazole moiety. It has to be noted that the respective rules were not explicitly derived for cleavage of phenolic rings bound to benzotriazole and therefore it is unknown if the mechanism proposed by UM-PPS is relevant in the environment.

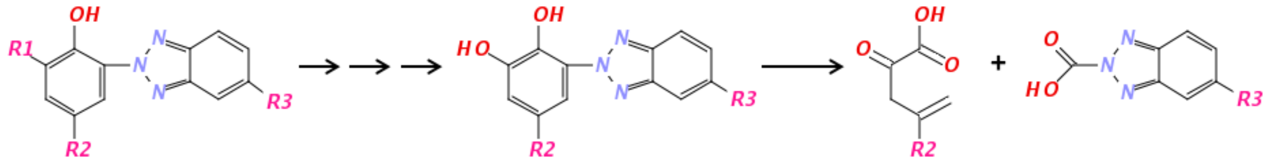


Figure 1: Proposed mechanism for the ring cleavage of the phenolic moiety of the phenolic benzotriazoles, R1: H, alkyl, aryl or alkyl-aryl; R2: alkyl, aryl or alkyl-aryl; R3: H or Cl. Side reactions are for the sake of simplicity not considered here.

In summary, with our current knowledge on the mechanism of the biodegradation of phenolic benzotriazoles, it seems reasonable to assume that they will be degraded slowly in the environment, especially if the position six is substituted with a complex side chain that has to be stepwise degraded. In case of UV-320 there is a tert-butyl group that is known to be hard to degrade as there is a quaternary carbon atom next to the aromatic ring.

To get a first impression on the actual potential for biodegradation, an estimation on the biodegradation behaviour was then done with BioWIN v4.10 (US EPA, 2011):

- Biowin2 (non-linear biodegradation probability) results in a value of 0.016 indicating that the substance does not biodegrade fast.
- Biowin6 (MITI non-linear biodegradation probability) results in a value of 0.0091 indicating that the substance is not readily degradable.
- Biowin3 (Survey model – ultimate biodegradation) results in a value of 2.1165 indicating that the degradation will take several months.

3.1.2.1.2 Screening tests

In a 28 day ready biodegradability test (performed according to the conditions of the test guidelines MITI I, OECD 301C; reliability rated Klimisch 2) using 100 mg/l of the substance and 30 mg/l sludge a degradation rate of 0 percent (BOD) was detected (NITE, 2012). Therefore the substance is expected to be not readily biodegradable. These results agree with the predictions of BIOWIN and the proposed complex degradation pattern.

3.1.2.1.3 Simulation tests

No simulation tests of the four phenolic benzotriazoles in question are available to us. However, dissipation and degradation of the substance EC 407-000-3 (Reaction mass of branched and linear C7-C9 alkyl 3-[3-(2-H-benzotriazol-2-yl)-5-(1,1-dimethyl)-4-hydroxyphenyl]propionates) in a water-sediment study according to OECD 308 was examined (dossier on 407-000-3). This substance is structurally related to the substances as it is a phenolic benzotriazole itself with a long-chained ester group in para-position to the hydroxyl group and a tert-butyl group in ortho-position. This study is used as further supporting information on degradation behaviour of the phenolic benzotriazoles.

Test conditions are generally well described and the test was done according to GLP. The report is reliable with restrictions (2 according to Klimisch).

As usual for this kind of study type two systems of different organic carbon content levels were employed. A river system contained low level and a pond system contained high level of organic carbon. Sampling locations of water and sediment were a pond and the river Rhine. For both systems the sampling locations were thought to not have been pre-exposed to the test substance or structural similar substances. The pond did not receive effluent discharge and this was assumed for the river Rhine, too, but as no exact sampling location was given some uncertainty remains. The test substance was radiolabelled in the benzene ring of the triazole moiety. Test systems were allowed to acclimatise for two weeks after filling. Test duration was 100 days and test temperature was 20 ± 2 °C. Water sediment ratio was 3.3:1. A stock solution which consisted of test substance in aceton was stepwise diluted to give a final concentration of the test substance of 3 µg/L. The test substance was applied dropwise onto the water surface. Water and sediment were separated and analysed at each sampling point. Two traps were employed for volatiles. On six occasions samples were taken and analysed. Analysis was done by TLC, HPLC and LSC and recovery rate was 98.7 % (96.2-101.2 %) for the river system and 99.9 % (97.6-101.9 %) for the pond system.

In both systems mineralisation was negligible with 1.2 or 1.3 % and the parent steadily declined to 3 or 4 % at day 100 in both systems. The steady decline hints on cometabolic degradation processes or abiotic degradation or dissipation processes. In neither system volatiles were detected. One metabolite (M1, CAS 84268-36-0) was identified, only. Thus a metabolic pathway could not be substantiated although it is clear that some degradation occurred that resulted in the metabolite M1.

The lack of mineralisation and the failed identification of further metabolites does not allow for differentiation of degradation and mere dissipation processes which contributed to the overall dissipation of M1. With no further metabolites identified adsorption and desorption of metabolites remain unknown. Dissipation may have been caused by mere adsorption. Another aspect that hampers differentiation is the relatively high level of non extractable residues (NER), because it remains unknown to which extent parent or metabolites contributed to NER formation.

M1 (see Figure 2) is the respective carboxylic acid of EC 407-000-3. It was detected as the main metabolite in quantities exceeding 10 % of the applied radioactivity by far and was found as well in the water as in the sediment phase. Twelve other metabolites were detected but not identified. Three metabolites reached amounts of 5 to 8 % in the total system at day 100.

In both systems M1 showed similar trends in the water phase. Here the maximum was reached at the third day with 15-20 % thereafter dropping below 10 % at day 28 which results in a DT_{50} < 40 days. According to Annex XIII a DT_{50} < 40 days would show M1 not to be persistent in water provided that DT_{50} would have been a $DegT_{50}$, but this cannot be stated with ample certainty.

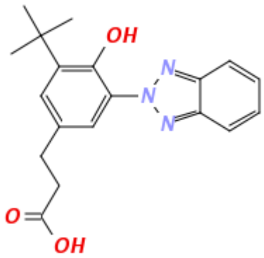


Figure 2: M1 (CAS 84268-36-0) is the first metabolite of degradation of EC 407-000-3

In the sediment phase the trend for M1 was similar in both systems up to day 14, afterwards it differed. After reaching a maximum a clear decrease was observed in the river system whereas only a slight decrease was observed in the pond system. In both systems the sediment values of M1 were already high at day 7 with 33 or 31 % of applied radioactivity and reached a similar high value on day 14 with 41 or 47 % (river or pond system). In the river system a maximum of approximately 47 % was reached at day 28 which finally decreased to 26 % at day 100. In the pond system an already high value of approximately 47 % on day 14 was followed by 34 % at day 28, reached a maximum of 56 % at day 56 and afterwards dropped only slightly to 50 % at test end on day 100.

Table 7 and Table 8 present the decline of M1 in the respective system taking the maximum value of M1 and the time at which maximum occurred as basis:

Table 7: Decline of M1 for sediment and whole system concentration in the river system (low org. C)

Sediment		**Whole system**	
Time in d	**Decline in %**	**Time in d**	**Decline in %**
0	0	0	0
28	20	14	2
72	46	42	27
		86	52

Table 8: Decline of M1 for sediment and whole system concentration in the pond system (high org. C)

Sediment		**Whole system**	
Time in d	**Decline in %**	**Time in d**	**Decline in %**
0	0	0	0
44	10	44	11

In the following an attempt is made to overcome the problem of a $DisT_{50}$ probably containing degradation as well as dissipation or partitioning processes by deduction of a $DegT_{50}$ from the specified $DisT_{50}$ for the purpose of comparing data with trigger values.

As stated above it is not possible to differentiate between degradation and mere dissipation processes, because of missing information on mineralisation and the unknown identities of the further metabolites and thus the $DisT_{50}$ of M1 for the sediment phase represents all processes. Another aspect that hampers differentiation is the relatively high level of non extractable residues (NER), because it remains unknown to which extent parent or metabolites contributed to NER formation. NER reached 36 % in the river system and 25 % in the pond system. They were mainly bound to the humic fraction and humic acids and to a lesser part to fulvic acids. Phenolic benzotriazoles have a high log K_{OC}. Therefore they have a high tendency to adsorb.

Though data are insufficient for kinetic modelling it is possible to draw the following conclusions: $DisT_{50}$ of M1 was approximately 72 days in river system which is well below the trigger DT_{50} < 120 days. As degradation shall be compared with the trigger value these dissipation data are improper for comparison purposes. It can be stated though, that $DegT_{50}$ will be longer than 72 days because it is only one of all the processes which contribute to the $DisT_{50}$.

Some further aspects should be considered which contribute to the overall picture. In the pond system only 11 % dissipation was reached in 44 days. It is impossible to derive a DT_{50} for the pond system, not even a $DisT_{50}$. It may only be stated that $DisT_{50}$ > 44 days in pond system. Nevertheless, a comparison with the river data shows that dissipation in the pond system in 44 days is only about half of the dissipation measured in the river system in 28 days which means dissipation was much slower in the pond system than in the river system.

Although it is not possible to extrapolate far beyond the available time frame the pond system data show that dissipation may be very slow depending on the conditions given.

Systems with high organic content generally should be more biologically active. They also have more potential binding sites for adsorption. The latter is thought to have been the case and would explain the different dissipation half-lives between the low and the high organic content systems.

In case of unclear contribution of partition processes to dissipation and if dissipation of the substance in question mainly takes place in sediment, the whole system data should be considered, too. Assessing the whole system ensures that mere adsorption will not have a decisive influence on a DT_{50} because adsorbed substance will show up in sediment.

The total occurrence of M1 (whole system) is mainly affected by M1 enrichment in sediment and consequently matches the course in sediment quite closely. Most important is the following lack of decline in the pond system.

In both systems the whole system values of M1 were already high at day 3, increased further and reached a similar high value on day 14. In the river system a maximum of approximately 55 % was reached at day 14 which only slightly decreased until day 28 but finally decreased to 26 % at day 100. In the pond system a near maximum of 56 % was reached at day 14, dropped afterwards to 39 % and raised again reaching finally a maximum of 57 % at day 56. It only decreased slightly to 51 % at day 100.

$DisT_{50}$ of M1 in the whole system was approximately 86 days in river system and more than 44 days in pond system. As degradation shall be compared with the trigger values these dissipation data are improper. Nevertheless, the fact that already dissipation half-life time is above 80 days means that $DegT_{50}$ will be longer.

Some further aspects should be considered which contribute to the overall picture. In the pond system only 11 % dissipation was reached in 44 days. A comparison with the river data within this time frame shows that this is only about half of the dissipation measured in the river system, i.e.

dissipation was much slower in the pond system than in the river system. Moreover, dissipation may have been even much slower than this. In pond system 56 % at day 14 was observed which is as nearly as high as the maximum of 57 % at day 56. Though the reported value is slightly lower it may also have been the same at both time points if one considers measuring inaccuracy. In this case 11 % of M1 would have been dissipated in 86 days.

A further test according to OECD 308 on degradation of EC 407-000-3 in water and sediment under anaerobic conditions was reported in the dossier on 407-000-3. Sediment was taken from an organic rich pond. In contrast to the aerobic test only small amounts of NER were found. With the exception of M1 all metabolites formed in small quantities, only. M1 reached 75 % in the whole system at day 100, 65 % were located in the sediment. Up to day 14 when the maximum of 32 % was reached the majority of M1 was found in the water phase. Afterwards the concentration decreased to 10 %. In the sediment phase concentration increased to the maximum of 65 % at test end. While EC 407-000-3 dissipated quickly its main metabolite M1 continuously built up throughout the test. Under anaerobic conditions M1 is persistent. We therefore conclude in a Read Across that the phenolic benzotriazoles in question will also be persistent.

Liu et al. (Liu et al., 2011a; reliability rated Klimisch 2) studied biodegradation of three different benzotriazoles under aerobic and varying anaerobic conditions to study degradation of these substances in wastewater treatment plants. For our assessment the substance 1H-Benzotriazole (CAS 95-14-7) is of importance, as it is a basic structural element of all phenolic benzotriazoles. Substance and metabolites were analysed by solid phase extraction followed by GC-MS and LC-MS/MS. Thus, primary degradation was measured only. A DT_{50} of 114 days was reported for aerobic conditions and a DT_{50} of 144 days was reported for anaerobic conditions. The study shows some deficiencies. The authors give insufficient information on test conditions. Additionally, the calculation model was not given.

They conclude that 1H-Benzotriazole was biodegraded slowly under the conditions given and report a DT_{50} of 114 d for aerobic and a DT_{50} of 144 d for anaerobic conditions. Keeping in mind the restricted reliability of the study data show that even under relatively favourable degradation conditions 1H-Benzotriazole is slowly degraded.

3.1.2.2 Biodegradation in sediments

Data from a Water-Sediment Test according to OECD 308 on the substance EC 407-000-3 (Dossier on 407-000-3) shows that sediment is a sink for the metabolite M1 (*cf.* 3.1.2.1.3). It is not possible to derive a $DegT_{50}$ but only a $DisT_{50}$ which is improper for comparison with the trigger values. This tentative $DisT_{50}$ is > 44 days or approximately 86 days depending on organic carbon content of the system for aerobic conditions. Under anaerobic conditions M1 was very persistent because it continuously built up throughout the test.

In marine and estuarine sediments in Japan UV-320 was detected in concentrations ranging from 0.3 to 2.3 ng/g dw (Nakata et al., 2009a). In polluted river sediments concentrations were 2.6 – 14 ng/g dw. These detections are of interest since UV-320 was banned in Japan as a Class I Specified Chemical Substance due to its PBT-properties since 2007 (Japan, 2007).

3.1.2.3 Biodegradation in soil

No data available.

3.1.2.4 Summary and discussion on biodegradation

Although there are no simulation tests on UV-320 itself, the results of the screening test as well as the result of simulation of these tests indicate a very low potential for biodegradation. The assumed degradation pathway is similar for all phenolic benzotriazoles and starts with a degradation of the side chains that are in ortho-position to the hydroxyl group of the phenolic ring. There is a simulation study on EC 407-000-3 which also gives information on a metabolite having a similar structure to the phenolic benzotriazoles in question. As it can be assumed that this phenolic benzotriazole will also be biodegraded according to the same mechanism and as it is structurally very similar to UV-320, we can use the results of this substance as a point for Read Across. Though it is impossible to compare data directly with the trigger values data give enough information to conclude that degradation will be slow or very slow under predominant aerobic conditions in environment. The same metabolite was constantly built up under anaerobic conditions and was hardly degraded at all. UV-320, which has also a tert-butyl group as side chain in ortho-position is at least as hard to degrade and will accordingly have a degradation half-life time that is at least as long.

The study of Liu et al. (2011) seems to support this theory further, as it shows that 1H-Benzotriazole itself already has a degradation half-life of over 100 days.

3.1.3 Summary and discussion on degradation

Biodegradation is expected to be the most relevant pathway for degradation of UV-320, if there is degradation. The overall evidence presented in chapter 3.1.2 in combination with the high-potential for adsorption on soil and suspended organic particles indicate in a Weight-of-Evidence-Approach that UV-320 will be persistent in the environment. This is to some extent supported by findings of UV-320 in the environment. Monitoring studies are available from Europe, USA and Asia demonstrating the presence of UV-320 in a variety of environmental samples including air, house and road dust, soil, surface water, sediments, aquatic organisms, WWTP influent, effluent and sludge, storm water, landfill effluent, combustible municipal solid waste and flue gas, fly ash and bottom ash of a pilot scale waste incinerator (see part II). However, the numbers of samples were small in these investigations and UV-320 was sometimes detected in few of the samples, only. Therefore the data have to be interpreted with caution. In addition there may be different uses of UV-320 and different amounts used in the different countries.

In soil UV-320 was detected in one of nine European samples at a concentration approaching 1 µg/g dw. The respective sampling site was a background site in Sweden. In sediments UV-320 was detected more often (Europe, Japan). Sediment concentrations ranged from a few ng/g dw to few µg/g dw. In Sweden even at background sites concentrations up to 0.56 µg/g dw were found. High concentrations at background sites may be interpreted as a proof of persistence. On the other hand the Swedish study is the only one with measured concentrations of that level. The authors of the study do not offer an explanation for this. It should also be noted that the detection limits for soil and sediments were very high in the Swedish study. In suspended solids from German river water (5 samples) UV-320 was not found.

3.2 Environmental distribution

3.2.1 Adsorption/desorption

As there is no registration dossier available QSAR-based calculations were performed to estimate the adsorption behaviour to soil or suspended organic matter for this substance. Details of the prediction can be found in Annex 3. The default input parameters were used.

Table 9: Results adsorption behaviour predictions of UV-320

Model	QSAR result	Overall model performance	QPREF
EPISuite 4.1 KOW-method	K_{OC} (L/kg): 4.30 10^4 Log K_{OC}: 4.63	Reliable with Restrictions	Annex 3.4
EPISuite 4.1 MCI-method	K_{OC} (L/kg): 1.17 10^5 Log K_{OC}: 5.07	Reliable with Restrictions	Annex 3.4
COSMOtherm	K_{OC} (L/kg): 1.48 10^5 Log K_{OC}: 5.17	Reliable with Restrictions	Annex 3.4

The results of the estimation of the adsorption behaviour lead to the conclusion that UV-320 will strongly adsorb to soil and organic suspended matter.

3.2.2 Volatilisation

The tendency for volatilization from the water phase was estimated by calculation of the Henry constant. Due to the absence of measured data on some physical-chemical properties an estimated melting point of 191 °C (result from MPBPWIN-module in EPISUITE v4.10; US EPA 2011) and a estimated water solubility of 0.1503 mg/l (result from WSkowWIN v1.42; US EPA 2011) were used for calculation of the Henry's law constant[3]. It was determined to be $4.884*10^{-3}$ $Pa*m^3*Mol^{-1}$ indicating only little tendency for volatilization. The air-water partitioning coefficient ($K_{air-water}$) may be derived from the Henry's law constant and is calculated to be $2.061*10^{-6}$ m^3/m^3. The $K_{air-water}$ and Henry's law constant are very low suggesting that volatilisation is unlikely to be a significant removal mechanism for UV-320 from aquatic systems and it is unlikely that the substance will be transported very far in the atmosphere (due to its atmospheric half-life estimated to be 9.534 hours).

3.2.3 Distribution modelling

Fugacity Level III distribution modelling

When released to the environment UV-320 will be distributed to the environmental compartments in different amounts. The table below shows the result of Fugacity Level III distribution modelling (Multiple Level III output) using EPI Suite v4.10 with the substance properties calculated within EPI Suite.

[3] according to equation R.16-4 from ECHA Guidance on Information requirements and Chemical Safety Assessment – Part R.16 (May 2010)

Table10: Distribution according to Mackay **Level III Fugacity Model (estimation with standard parameters as provided by EPI Suite v4.10)**

compartment	**mass amount (percent)**
air	$2.37*10^{-5}$
water	4.73
soil	63.3
sediment	32.3

The results of the distribution modelling and physical-chemical substance properties lead to the conclusion that the overall amount of the substance will adsorb to the soil (63.3%) and the sediment (32.3%).

The dominant route of exposure for UV-320 is expected to be wastewater which is treated in sewage treatment plants. Therefore calculations based on physical-chemical data retrieved from QSAR have been used to estimate the distribution of the substance in sewage treatment plants with the help of SimpleTreat. The calculation was done assuming that the substance is not biodegradable (k=0/h).

Table 11: Distribution in sewage treatment plants (acc. To SimpleTreat 3.0, debugged version; 7 Feb 1997)

Summary of distribution	**percent**
to air	0.0
to water	9.5
via primary sludge	65.6
via surplus sludge	25.0
Degraded	0.0
Total	*100*

The results of the calculation lead to the conclusion that when UV-320 is released into waste water, the largest part of the substance will be held back in the sewage sludge and does not enter the environment. This is in agreement with experimental findings (see Part 2 and Annex 3). It has to be kept in mind that the use of sludge from municipal sewage treatment plants for agricultural proposes is a common practice in many regions. Over this pathway of exposure the substance might be released into agricultural soil.

3.3 Bioaccumulation

To our knowledge there are no experimental log K_{OW}-values for UV-320. Therefore we calculated the value with the QSAR model KOWWIN of EPISuite 4.10 and with COSMOtherm. Details on these calculations can be found in Annex 4.

Table 12: QSAR-Results for log K_{OW}-predictions of UV-320

Model	QSAR result	Overall model performance	QPREF
EPISuite 4.1 KOWWIN	Log K_{OW}: 6.27	Reliable	Annex 4.3
COSMOtherm	Log K_{OW}: 7.39	Reliable	Annex 4.3

Based on the estimated log K_{OW}-values that are larger than 4.5, it is expected that UV-320 will bioaccumulate.

3.3.1 Aquatic bioaccumulation

The German UBA re-evaluated a test on UV-320 according to MITI guideline (OECD 305 C) based on excerpts of the original test protocol which was made available by NITE (NITE, 2012; reliability rated Klimisch 2).

Test duration was 14 weeks except for the test with a concentration of 0.1 µg/L where it was only 10 weeks. Not all test conditions can be reported because the summary of the studies does not list them.. For example no information on the use of a dispersant is given, but in two similar studies on UV-327 which has also a low water solubility dispersants were used.

In general, the data of the three test concentrations 10.0, 1.0 and 0.1 µg/L show similar trends although maximum BCF values are less than or above 2000 for the highest test concentration and well above 2000 for the other two test concentrations (*cf.* Table 13).

Data of all test concentrations show a quite steady increase of BCF over a longer time frame of 10-12 weeks until a maximum is reached. Some variability is observed in each data row (two parallel samples per sampling time point for each concentration) but we do not believe that this renders the data not reliable. It rather reflects difficulties which are observed in many cases with substances of low water solubility.

A BCF of 2250 was measured in one data row of the highest test concentration in week 10, but dropped to 703 in week 12 and raised again to 1540 in week 14. As there is no explanation for this unusual trend these data should be treated as not reliable. The second data row is the only one to show a steady state with an average BCF of 1473 (single values 1570, 1510 and 1340).

Neither of the data rows of the medium or the low test concentration reaches steady state. BCF data for the medium concentration reach a maximum at week 10 or 12 and drop again at week 14. BCF data for the lowest test concentration reach a maximum at week 8 or 10 at which time the test ended.

A comparison of BCF data of the three test concentrations shows a trend of higher BCF values with lower test concentrations. Such trends are common in cases in which the test concentration in water is overestimated. Considering the calculated water solubility of 0.15 mg/L this is not believed to have had an influence in the test, though.

It is concluded that the test is reliable though no steady state was reached with the above mentioned one exception. Thus for the assessment the maximum BCF values and the values at the test end should be considered. Maximum BCF values represent the worst case and the BCF at test end represent a best case for the high and medium concentration because probably some elimination had already started.

For two of the three concentrations tested both maximum value and BCF at test end clearly are above the trigger value of 2000 and also above 5000 when lipid normalised.

Table 13: Compilation **of BCF maxima and BCF values at test end (values refer to whole body wet weight basis unless no other information is provided)**

Test concentration in µg/L	Maximum BCF measured	Maximum BCF normalised to 5% lipid content	average BCF measured at test end	BCF at test end normalised to 5% lipid content
10	2250[1] 1473[1]	3040 1990	1440	1945
1	7785[1]	10520	4370	5905
0.1	9265[2]	12868	8670	12041

[1] Lipid content of test fish 3.7 %

[2] Lipid content of test fish 3.6 %

3.3.2 Terrestrial bioaccumulation

No data available.

3.3.3 Summary and discussion of bioaccumulation

For two of three test concentrations BCF are above the vB trigger of 5000. There is a trend of higher BCF values with lower test concentration. This trend is frequently observed if concentration of the test substance in water is overestimated. All test concentrations are well below the water solubility, though, so this effect is not probable here and should not have influenced the results. Even if the suspicion should be true it would not render the study results worthless because in this case BCF would have been underestimated and the real BCF would have been even higher. Thus, data show UV-320 to meet the vB criterion.

Monitoring data on UV-320 in biota are available from Sweden, USA and Asia (see part II). UV-320 was not detected in 4 fish samples from Sweden (high detection limit of 0.9 µg/g dw), in 2 liver samples of water fowl and 5 samples of marine mammals (blubber) from Japan and in mussel samples from the USA and 9 Asian countries. It was found in 51 of 63 marine fish samples from the Philippines and in 9 of 10 marine tidal flat organisms and 5 of 16 marine shallow water organisms from Japan. Concentrations up to 74 ng/g lw were detected. UV-320 is especially found in lipid of lower benthic organisms collected from tidal flat areas. In 4 of 7 mussel samples from Japan up to 86 ng/g lw were detected. UV-320 also seems to be accumulated in the liver of some fish. In summary monitoring data on UV-320 can only give a certain indication that bioaccumulation may occur.

However, data for structural similar substances support the vB conclusion. For UV-327 a lipid-normalised BCF of 8817 and for UV-350 lipid-normalised BCF of 20263 and 34210 was shown. Additionally, a lipid-normalised field BAF of 5946 for UV-327 and a lipid-normalised field BAF of

6429 for UV-328 were found in a monitoring study by Nakata (Nakata et al., 2010). Biomonitoring studies suggest a strong dependency of the bioaccumulation potential of phenolic benzotriazoles on the species considered. Also enrichment in top predators is at least in some cases suggested (see Annex 5).

Table 14 gives an overview over the available data on bioconcentration on all four phenolic benzotraizoles discussed.

Table 14: Overview of the available data on bioconcentration properties of UV-320, UV-327, UV-328 and UV-350 (values refer to whole body wet weight basis unless no other information is provided)

Substance	Species	BCF/BAF (lipid norm.)	c [µg/L]	Test system	Type	References
UV-320	*Cyprinus carpio*	1,945*	10	OECD 305C	kinetic	(NITE, 2012)
		5,905*	1			
		12,041*	0.1			
UV-327	*Cyprinus carpio*	1,203	1.0	OECD 305C	steady state	(NITE, 2012)
		6,283	0.1			
		8,817	0.1			
		7,540	0.01			
	Neophocaena phocaenoides	5,946	0.012 **	Monitoring	-	(Nakata et al, 2010)
UV-328	*Cyprinus carpio*	1,121	0.1	OECD 305C	steady state	(NITE, 2012)
		740-2,148	0.01			
		3,681	0.01			
	Neophocaena phocaenoides	6,429	0.012 **	Monitoring	-	(Nakata et al, 2010)
UV-350	*Cyprinus carpio*	20,263	1.0	OECD 305C	steady state	(NITE, 2012)
		34,210	0.1			

* at test end

** geometric mean concentration reported by Ministry of Environment, Japan

3.4 Secondary poisoning

UV-320 is expected to enrich in top predators because accumulation through the food chain was shown for the structural similar UV-327 and UV-328. Several biomonitoring studies suggest that as well (see Annex 5).

4 HUMAN HEALTH HAZARD ASSESSMENT

4.1 Repeated dose toxicity

4.1.1 Non-human information

4.1.1.1 Repeated dose toxicity: oral

In an oral subacute toxicity study, UV-320 produced liver toxicity and changes in haematological and clinical chemistry parameters in male rats already at the lowest dose level of 0.5 mg/kg bw/d. At dose levels ≥ 2.5 mg/kg bw/d, vacuolar degeneration of hepatocytes and focal necrosis in the liver were reported.

In female rats, liver toxicity was observed at doses of 12.5 mg/kg bw/d and higher. Only the highest dose increased glucose, the A/G ratio, total cholesterol, triglycerides and ALT (see table 4.6.1.1).

Additional effects were observed in both sexes in the heart, where doses of 12.5 mg/kg bw/d and higher induced degeneration and/or hypertrophy of the myocardium. Finally, effects were noted in kidney, thyroids and the spleen (diffuse follicular cell hyperplasia in both sexes at doses of 62.5 mg/kg bw/d).

After the 14-day recovery period, these changes mostly recovered in females, but not in males.

The LOAEL for male rats was 0.5 mg/kg bw/day. A NOAEL of 2.5 mg/kg bw/day was derived for female rats.

In the follow-up, an oral subacute toxicity study was performed with castrated rats. As shown in the previous study clinical chemistry parameters were influenced already at the lowest dose level of 0.5 mg/kg bw/d. Histopathology was only investigated in liver and heart. Only in the liver effects were observed: At 0.5 mg/kg bw/day and above a diffuse hypertrophy of hepatocytes was found in the liver of male rats with anisokaryosis, nucleolar enlargement and decreased glycogen (see table 16). Similar effects were observed in the liver of female rats treated with 2.5 mg/kg bw/day and above. In addition, focal coagulative necrosis at 12.5 mg/kg bw/day in males and at 2.5 mg/kg bw/day and above in females were detected.

The LOAEL for male and female rats was 0.5 mg/kg bw/day. Castration markedly reduced gender-related differences in the toxicity of UV-320 in male and female rats.

In an oral subchronic toxicity study, UV-320 influenced some haematological parameters as well as clinical chemistry parameters (see table 16). On histopathology, centrilobular hypertrophy of hepatocytes, accompanied with eosinophilic granular cytoplasm was observed in the liver. The incidence was significantly increased at 2.5 mg/kg bw/day in males and at 12.5 mg/kg bw/day in females.

In an oral chronic toxicity study, UV-320 influenced some haematological parameters as well as clinical chemistry parameters (see table 16). Liver was enlarged in male rats already at dose levels of 0.5 mg/kg bw/day. As observed at the end of the 13-week administration period, centrilobular hypertrophy of hepatocytes with eosinophilic granular cytoplasm was observed on histopathological examination, and the incidence was significantly increased at 0.5 mg/kg bw/day and higher in males, and at 12.5 mg/kg bw/day in females (see table 16). In addition, significant increases in the incidence of cystic degeneration and lipofuscin deposition in hepatocytes at 2.5 mg/kg bw/day, and of altered hepatocellular foci (clear cell foci) at 0.5 mg/kg bw/day and higher were found in the liver of males.

Table 15: Overview of the key study for repeated dose toxicity

Method	Results	Remarks	Reference
28 day repeated dose toxicity test in mammalian species Crj:CD(SD) rats male/female 10 males/females in control and the highest dose group, and 5/sex in other dose groups UV-320 in corn oil by gavage Doses: 0.5, 2.5, 12.5, 62.5 mg/kg bw/day Control: corn oil only 5 rats/sex in control and the highest dose group were investigated after a recovery period of 14 days	No mortality No effects on body weight and weight gain Increase in food consumption on dosing days 14 and 21 in males and on dosing days 21 and 27 in females at 62.5 mg/kg bw/day Haematology At ≥ 2.5 mg/kg bw/d (m) decrease in red blood cell count, haematocrit and haemoglobin. At ≥ 12.5 mg/kg bw/d (m) decrease in MCHC At 62.5 mg/kg bw/d (m) increases in platelet count Clinical chemistry At ≥ 0.5 mg/kg bw/d (m) increase in A/G ratio At ≥ 2.5 mg/kg bw/d (m) increase in glucose At ≥ 12.5 mg/kg bw/d (m) increase in albumin, ALT and ALP At ≥ 62.5 mg/kg bw/d (m) increase in BUN and AST At ≥ 62.5 mg/kg bw/d (f) increase in glucose, A/G ratio, total cholesterol, triglyceride and ALT Organ weights At ≥ 0.5 mg/kg bw/d (m) increase in relative liver weight At ≥ 2.5 mg/kg bw/d (m) increase in absolute liver weight At ≥ 12.5 mg/kg bw/d (f) increase in absolute and relative liver weight At 62.5 mg/kg bw/d (m) increase in absolute and relative kidney weight At 62.5 mg/kg bw/d (f) increase in absolute heart weight Gross pathology At ≥ 0.5 mg/kg bw/d (m) enlargement of the	1 (reliable without restriction) key study experimental result	Hirata-Koizumi et al., 2007

	liver At ≥ 2.5 mg/kg bw/d (m) white patch/zone in the liver At ≥ 12.5 mg/kg bw/d (f) enlargement of the liver At 62.5 mg/kg bw/d (f) white patch/zone in the liver <u>Histopathology</u> <u>Liver</u> At ≥ 0.5 mg/kg bw/d (m) hypertrophy of hepatocytes and bile duct proliferation and decreased incidence of hepatocellular fatty change At ≥ 2.5 mg/kg bw/d (m) vacuolar degeneration of hepatocytes and focal necrosis At ≥ 12.5 mg/kg bw/d (f) hypertrophy of hepatocytes and focal necrosis At 62.5 mg/kg bw/d (m) hepatocellular pigmentation and/or cytoplasmic inclusion bodies At 62.5 mg/kg bw/d (f) bile duct proliferation and decreased incidence of hepatocellular fatty change and vacuolar degeneration of hepatocytes At 62.5 mg/kg bw/d (m+f) increased mitosis of hepatocytes Heart At ≥ 2.5 mg/kg bw/d (m) cell infiltration At ≥ 12.5 mg/kg bw/d (m+f) degeneration and/or hypertrophy of myocardium Kidney At ≥ 12.5 mg/kg bw/d (m) hypertrophy of the tubular epithelium At 62.5 mg/kg bw/d (m) increased severity of basophilic tubules At 62.5 mg/kg bw/d (f) hypertrophy of the tubular epithelium Thyroid At 62.5 mg/kg bw/d (m+f) diffuse follicular cell hyperplasia Spleen At ≥ 2.5 mg/kg bw/d (m) extramedullary		

	haematopoiesis At 62.5 mg/kg bw/d (m+f) diffuse follicular cell hyperplasia		

4.1.2 Summary and discussion of repeated dose toxicity:

In an oral subacute toxicity study, UV-320 showed toxicity in several organs. Target organ in male rats was the liver with first effects (hypertrophy of hepatocytes and bile duct proliferation) at the lowest dose of 0.5 mg/kg bw/d already. Males receiving doses of 2.5 mg/kg bw/d and higher displayed vacuolar degeneration of hepatocytes and focal necrosis.

Further studies with lower dosage levels (subchronic and chronic) confirmed these results and underlined the hepatotoxic properties of UV-320.

These effects meet the criteria of Regulation EC 1272/2008 (CLP), Annex I, section 3.9.2.7.3 (d) for classification for ’Specific target organ toxicity – repeated exposure’. Moreover, as the LOAEL for these findings is < 10 mg/kg bw/d, the subcategory STOT RE 1 could be assigned, in line with CLP Annex I, Table 3.9.2.

In conclusion, based on the provisions of Annex XIII, section 1.1.3 (c) of the REACH Regulation, UV-320 meets the T-criterion.

5 ENVIRONMENTAL HAZARD ASSESSMENT

5.1 Aquatic compartment (including sediment)

5.1.1 Toxicity data

5.1.2 Toxicity data

5.1.2.1 Fish

5.1.2.1.1 Short-term toxicity to fish

In 2007 a study was presented under the Existing Chemicals Law of Japan where in a 48 h acute toxicity test a LC_{50} of >500 mg l^{-1} was reported.

Table 16: Acute toxicity of UV-320 on fish.

Species	**Duration**	**LC_{50} (mg l^{-1})**	**Method, conditions**	**Rel.**	**Reference**
Oryzias latipes	48 h	>500	Japanese Industrial Standard (JIS K 0102-1993-71.)	4	(Japan, 2007a,)

5.1.2.1.2 Long-term toxicity to fish

No data relevant for assessing the T-criterion can be reported.

5.1.2.2 Aquatic invertebrates

5.1.2.2.1 Short-term toxicity to aquatic invertebrates

There is a recent study by Kim et al. testing the acute toxicity of the Benzotriazole UV-stabilizers UV-9, UV-234, UV-320, UV-326, UV-327, UV-328, UV-329, UV-360 and UV-571. The tests were conducted according to the OECD Testing Guideline 202 on *Daphnia Pulex* in different concentrations up to 10 mg l^{-1} (Kim et al., 2011a). Only for UV-571 acute toxic effects were reported with an LC_{50}(24h) of 6.35 mg l^{-1} and an LC_{50}(48 h) of 2.59 mg l^{-1}. For all the other stabilizers no toxic effects were observed under the concentrations tested in the study.

Table 17: Short-term-toxicity of UV-320 on aquatic invertebrates.

Species	**Duration**	**EC_{50} (mg l^{-1})**	**Method, conditions**	**Rel.**	**Reference**
Daphnia Pulex	24 h	>10	OECD TG 202	1	(Kim et al., 2011a)
Daphnia Pulex	48 h	>10	OECD TG 202	1	(Kim et al., 2011a)

5.1.2.2.2 Long-term toxicity to aquatic invertebrates

No data relevant for assessing the T-criterion can be reported.

5.1.2.3 Algae and aquatic plants

No data relevant for assessing the T-criterion can be reported.

5.1.2.4 Sediment organisms

No data relevant for assessing the T-criterion can be reported.

5.1.2.5 Other aquatic organisms

No data relevant for assessing the T-criterion can be reported.

5.2 Terrestrial compartment

No data relevant for assessing the T-criterion can be reported.

5.3 Atmospheric compartment

No data relevant for assessing the T-criterion can be reported.

5.4 Microbiological activity in sewage treatment systems

No data relevant for assessing the T-criterion can be reported.

5.5 Non compartment specific effects relevant for the food chain (secondary poisoning)

5.5.1 Toxicity to birds

No data relevant for assessing the T-criterion can be reported.

5.5.2 Toxicity to mammals

See Chapter 4.6

5.6 Toxicity test results concerning endocrine disruption relevant for the environment

As there is some discussion on endocrine disrupting properties data on this issue was compiled in Annex 6.

6 CONCLUSIONS ON THE SVHC PROPERTIES

6.1 PBT, vPvB assessment

6.1.1 Assessment of PBT/vPvB properties – comparison with the criteria of Annex XIII

6.1.1.1 Persistence

If UV-320 is degraded, biodegradation is expected to be the most relevant pathway for degradation. Although there are no simulation tests on UV-320 itself, based on a Weight-of-Evidence argumentation it can be demonstrated that UV-320 is very persistent. This argumentation is based on the following facts;

- In many environmental monitoring studies UV-320 is analysed in a variety of different compartments in many regions of the world (see Annex 5). In Japanese studies from 2009 findings of UV-320 were analysed. The substance was found (in lower concentrations) although it is banned in Japan as a Class I Specified Chemical Substance due to its PBT-properties since 2007 (Japan, 2007).

- Once released into the environment, most UV-320 will be bound to soil or sediment as the substance has a very high potential for adsorption. This was demonstrated by experimental results on sewage sludge as well as simulated log K_{OC} values.

- The results of the screening test on ready biodegradation as well as the result of simulation of this tests indicate a very low potential for biodegradation

- In the common mechanism for degradation of phenolic benzotriazoles the side-chain in ortho-position is degraded first. The more complex this side chain is, the longer it will take for the respective substance to be degraded. In case of UV-320 a tert-butyl group has to be degraded.

- While the single available simulation study using EC 407-000-3, a similar substance with also a tert-butyl group in ortho-position, does not allow a direct comparison of data with the trigger values, it shows that even dissipation of one metabolite is slow. Thus degradation will be even slower. This metabolite is hardly degraded at all under anaerobic conditions. Considering the high potential for adsorption these conditions are expected to be important substance sinks.

- Additional information exist for the basic structure of the phenolic benzotriazole, i.e. 1H-benzotriazole. Under favourable degradation conditions of a simulated waste water treatment plant a degradation half-life time of over 100 days is reported.

In conclusion it is therefore assessed that UV-320 must be considered to be very persistent in the environment.

6.1.1.2 Bioaccumulation

UV-320 shows very high bioconcentration with BCF above the vB trigger of 5000. This finding is in line with BCF of the other benzotriazoles UV-327 and 350, the latter one's BCF exceeding the trigger by far. Additionally, enrichment at the top of the food chain has been proven for UV-327 and UV 328. Thus UV-320 is very bioaccumulative.

6.1.1.3 Toxicity

The available studies show that UV-320 is not acutely toxic for aquatic organisms. There is no information on the long-term toxicity of UV-320. However, in an oral subacute toxicity study, UV-320 showed toxicity in several organs. Target organ in male rats was the liver with first effects (hypertrophy of hepatocytes and bile duct proliferation) at the lowest dose of 0.5 mg/kg bw/d already. Males receiving doses of 2.5 mg/kg bw/d and higher displayed vacuolar degeneration of hepatocytes and focal necrosis.

These effects meet the criteria of Regulation EC 1272/2008 (CLP), Annex I, section 3.9.2.7.3 (d) for classification for 'Specific target organ toxicity – repeated exposure'. Moreover, as the LOAEL for these findings is < 10 mg/kg bw/d, the subcategory STOT RE 1 has to be assigned, in line with CLP Annex I, Table 3.9.2.

In conclusion, based on the provisions of Annex XIII, section 1.1.3 (c) of the REACH Regulation, UV-320 meets the T-criterion.

6.1.2 Summary and overall conclusions on the PBT, vPvB properties

UV-320 has to be considered vP and therefore also P. Also the substance fulfils the numerical criterion to be considered vB and therefore also B. Finally, UV-320 fulfils also the criteria to be classified as STOT-RE 1 and therefore can be considered as toxic. In conclusion UV-320 has vPvB- and PBT-properties.

6.2 CMR assessment

Not relevant for this dossier.

Part II

INFORMATION ON USE, EXPOSURE, ALTERNATIVES AND RISKS

INFORMATION ON MANUFACTURE, IMPORT/EXPORT AND USES

Phenolic benzotriazoles are used as UV-stabilizers since they can absorb the full spectrum of UV-light: UV-A (320-400 nm) and UV-B (280-320 nm). Beside the group of benzophenones, they are technically the most important UV-absorbers, especially for transparent plastic materials. The different phenolic benzotriazoles have different substitution patterns in ortho- and para-position to the hydroxyl group of the phenolic ring. This difference has effects on the solubility and the distinct coloration in different transparent plastic materials (Kirk et al., 2007).

According to the personal communication with a big globally acting producer of chemicals approximately 50% of all of their products of this substance class are used as UV-protection agents in coatings especially for cars and special industrial wood coatings. Ca. 40% are used as UV-protection agents for plastics, rubber and polyurethanes. The rest is used in cosmetics (e.g. as sun protection agents). We do not know if the percentages are representative for industry in general, but the uses seem to be limited to these fields of application.

UV-320 is preregistered and the number of individual notifications in ECHA's C&L Inventory database[4] (total number: 128, subdivided into 6 different aggregated notifications) leads to the conclusion that UV-320 is commercially relevant inside Europe.

Concerning tonnages manufactured or imported we do not have a complete picture of the situation yet, as UV-320 is not registered under REACH at the moment. It is expected that companies will register UV-320 within the second registration phase until 31. May 2013 in the tonnage band 100 to 1000 tonnes per year because no registration until 30. November 2010 was carried out. It has to be kept in mind that the registration only covers a single registrant. Even when only 6 aggregated notifiers of the C&L inventory might submit a registration dossier for a tonnage band 100 – 1000 tonnes per year the aggregated tonnages over all registrants might exceed threshold of 1000 tonnes per year without circumstances.

According to our general knowledge on phenolic benzotriazoles, we expect that the substance itself will be used as UV-stabilizer for plastics, polyurethanes and rubber and constituent in formulations used for coating of surfaces, e.g. cars or special industrial wood coatings.

Consultation of the database of Substances in Products in Nordic Countries[5] (SPIN) refers to 13 preparations containing UV-320 in a total quantity around 1.0 tonnes per year (reporting year: 2010). But this information is expected not to be excessive because the data reported by Finland is

[4] http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database; (accessed 15th February 2013)

[5] Information from SPIN-database (www.spin2000.net; accessed 20th July 2012)

claimed to be confidential. The reported types of preparations where UV-320 is a constituent are adsorbents used for the manufacture of rubber and plastic products.

EXPOSURE

Releases to the environment

Because there was no registration under REACH for UV-320 in the first registration phase at the moment no information on releases and environmental exposure from Chemical Safety Reports is available.

Measured releases

Measured concentrations in the environment

UV-320 was found in three air samples in Sweden in concentrations below 1 ng/m³ (Brorström-Lundén et al., 2011). It was present in a background sample as well as in some potentially polluted sites. In samples of air deposition no UV-320 was detected (< 100 ng/m² day). UV-320 was detected in most house dust samples from Manila (Kim et al., 2012). The median concentration in dust from a residential area was 4.7 ng/g, the maximum 25 ng/g. UV-320 was also detected in road dust in Japan with concentrations from ca. 0.7 to ca. 3 ng/g dw (Nakata et al., 2011).

One of four Swedish soil samples contained UV-320 in a concentration of 0.91 µg/g dw, whereas the concentration in three other samples was below 0.4 µg/g dw (Brorström-Lundén et al., 2011). In Germany UV-320 was not detected in 3 soils with high anthropogenic influence and 2 soils from background sites (Rodríguez Pereiro and Casado Agrelo, 2012).

In some Swedish surface water samples UV-320 was detected in concentrations below 1 ng/L (Brorström-Lundén et al., 2011). In Germany UV-320 could not be detected in 5 samples of suspended particulate matter from river water independent of the anthropogenic influence at the sampling site (Rodríguez Pereiro and Casado Agrelo, 2012).

Sediment samples contained UV-320 in the range of 0.13-3 µg/g dw. (Carpinteiro et al., 2012a) found UV-320 in one of ten European sediments at a concentration of 5.6 ng/g. In marine and estuarine sediments in Japan UV-320 was detected in concentrations ranging from 0.3 to 2.3 ng/g dw (Nakata et al., 2009a). In polluted river sediments concentrations were 2.6 – 14 ng/g dw.

UV-320 was neither detected in treated industrial wastewater of an American specialty chemicals manufacturing plant, nor in the receiving Pawtuxet River water, but in sediments (40 ppm) (Jungclaus et al., 1978).

Concentrations of UV-320 in (few) Swedish fish samples were below the detection limit of 0.9 µg/g dw (Brorström-Lundén et al., 2011). In 9 of 10 species of marine tidal flat organisms from Japan (n = 19) UV-320 was present at concentrations of 0.07 – 0.60 ng/g ww (Nakata et al., 2009a). Based on lipid weight highest concentrations were found in tidal flat clam (74 ng/g lw). In 2 of 10 species of marine shallow water organisms (n = 18) concentrations were lower (0.06 and 0.09 ng/g ww), whereas in the liver of 3 of 6 species of shallow water organisms (n = 13) higher concentrations were detected (0.41 – 7 ng/g ww). In the liver of spot-billed duck and mallard concentrations were <0.05 ng/g ww. A further study on marine organisms from Japan confirms that UV-320 is especially found in lipid of lower benthic organisms collected from tidal flat areas (Nakata et al., 2009b). UV-320 also seems to be accumulated in the liver of some fish. In blue and green mussels from 10 Asian countries UV-320 was detected in several mussels from Japan, only (Nakata et al., 2012). Concentrations ranged from 39-86 ng/g lw in four of seven samples. UV-320 was not detected in the blubber of finless porpoises in Japan (Nakata et al., 2010). In fish muscle samples from the Philippines (3 species, n = 5) UV-320 was present in concentrations ranging from 0.78 to 9.6 ng/g lw (Kim et al., 2011b). In a further study on 20 species (n = 58) UV-320 was detected in 79% of the samples. Concentrations ranged from n.d. to 28.7 ng/g lw (Kim et al., 2011c). Concentrations in the different fish species varied greatly. The highest concentrations were found in fish from demersal habitat.

Carpinteiro et al (Carpinteiro et al., 2012b) detected UV-320 in one sample of raw wastewater of a Portuguese WWTP (24 ng/L), but not in Spanish wastewater samples. UV-320 was not detected in treated wastewater of the WWTPs. In Sweden one of five WWTP effluents (4 ng/L) and six of eight WWTP sludges (0.84-2 µg/g dw) contained UV-320 (Brorström-Lundén, 2011). In particles of WWTP effluent UV-320 was below the detection limit of 61 µg/g dw. In Japan UV-320 was not detected in influent, effluent and sewage sludge samples from five WWTPs (Nakata and Shinohara, 2010). In China no UV-320 was found in 60 samples of municipal WWTP sludge (Ruan et al., 2012).

Brorström-Lundén et al. (2011) found UV-320 in two of three landfill effluents (7.3 and 23 ng/L) and one of four storm water samples (0.73 ng/L). Particles of a landfill effluent sample contained UV-320 below the detection limit of 0.7 µg/g dw.

Concentration of UV-320 in “refuse derived fuels” obtained from Japanese municipal solid waste after removing the incombustible materials was 7.1 ng/g (Watanabe and Noma, 2010). After treatment in a pilot-scale incinerator the concentration in the flue gas (final exit) was 0.0020 µg/m^3. Bottom ash contained 0.52 ng/g UV-320, fly ash 0.36 ng/g. This study was conducted after the ban of UV-320 for most uses in Japan.

Table 18: Overview of UV-320 detections in the environment

Compartment	**Concentration**	**Detection frequency**	**Country of sampling**	**Reference**
air	0.024 and 0.67 ng/m³ background sites: 0.44 ng/m³	2/6* 1/2	Sweden	(Brorström-Lundén et al., 2011).
air deposition	n.d. background sites: n.d.	0/2 0/2	Sweden	(Brorström-Lundén et al., 2011).
house dust	median 4.7 ng/g max. 25 ng/g (residential area)	30/37	Philippines	(Kim et al., 2012).
road dust	ca. o.7 - ca. 3 ng/g dw	7/9	Japan	(Nakata et al., 2011).
soil	n.d. background site: 0.91 µg/g dw	0/3 1/1	Sweden	(Brorström-Lundén et al., 2011).
	n.d. (2 background sites , 3 sites with high anthropogenic influence)	0/5	Germany	(Rodríguez Pereiro and Casado Agrelo, 2012)
surface water	0.68 and 0.94 ng/L background sites: 0.55 ng/L	2/4 1/2	Sweden	(Brorström-Lundén et al., 2011).
	n.d. (industrial pollution)	0/16	USA	(Jungclaus et al., 1978).
suspended solids (from river water)	n.d. (background sites, sites with high anthropogenic influence)	0/5	Germany	(Rodríguez Pereiro and Casado Agrelo, 2012)
sediment	0.18 - 3 µg/g dw background sites: 0.16 and 0.56 µg/g dw	3/3 2/3	Sweden	(Brorström-Lundén et al., 2011).
	5.6 ng/g	1/10	Europe	(Carpinteiro et al., 2012a)
	2.6 – 14 ng/g dw (polluted river)	5/5	Japan	(Nakata et al., 2009a).
	40 ppm (industrial pollution)	1/19 ?	USA	(Jungclaus et al., 1978).
marine sediment	0.3 – 2.3 ng/g dw	11/11	Japan	(Nakata et al., 2009a).
fish	n.d. background sites: n.d.	0/2 0/2	Sweden	(Brorström-Lundén et al., 2011).
marine fish	0.78 - 9.6 ng/g lw	5/5	Philippines	(Kim et al., 2011b)
	max. 28.7 ng/g lw	46/58	Philippines	(Kim et al., 2011c).

marine tidal flat organisms (incl. fish)	0.07 – 0.60 ng/g ww max. 74 ng/g lw	9/10 species	Japan	(Nakata et al., 2009a).
mussels	39 - 86 ng/g lw mean 33 ng/g lw geometric mean 13 ng/g lw	4/7	Japan	(Nakata et al., 2012)
	n.d.	0/2	Cambodia	
	n.d.	0/5	China	
	n.d.	0/8	Hong Kong	
	n.d.	0/3	India	
	n.d.	0/2	Indonesia	
	n.d.	0/17	Korea	
	n.d.	0/4	Malaysia	
	n.d.	0/2	Philippines	
	n.d.	0/15	USA	
	n.d.	0/3	Vietnam	
marine shallow water organisms (incl. fish)	2 species: 0.06 and 0.09 ng/g ww 3 species in liver: <0.05 – 7 ng/g ww	5/16 species	Japan	(Nakata et al., 2009a).
water fowl	liver: n.d.	0/2 species	Japan	(Nakata et al., 2009a).
marine mammals	n.d. in blubber	0/5	Japan	(Nakata et al., 2010)
wastewater	24 ng/L n.d.	1/1 0/2	Portugal Spain	(Carpinteiro et al., 2012b)
	n.d.	0/5	Japan	(Nakata and Shinohara, 2010)
WWTP effluent	4 ng/L particles: n.d.	1/5 0/1	Sweden	(Brorström-Lundén et al., 2011).
	n.d. n.d.	0/1 0/2	Portugal Spain	(Carpinteiro et al., 2012b)
	n.d.	0/5	Japan	(Nakata and Shinohara, 2010)
	n.d. (industrial WWTP)	?	USA	(Jungclaus et al., 1978).
WWTP sludge	0.84 - 2 µg/g dw	6/8	Sweden	(Brorström-Lundén et al., 2011).
	n.d.	0/60	China	(Ruan et al., 2012).
	n.d.	0/5	Japan	(Nakata and Shinohara, 2010)
storm water	0.73 ng/L	1/4	Sweden	(Brorström-Lundén et al., 2011).
refuse derived fuel (combustible municipal solid waste)	7.1 ng/g	1/1	Japan	(Watanabe and Noma, 2010).
landfill effluent	7.3 and 23 ng/L particles: n.d.	2/3 0/1	Sweden	(Brorström-Lundén et al., 2011).
pilot-scale flue gas	2 ng/m³	1/1	Japan	(Watanabe and Noma, 2010).

waste incinerator	fly ash	0.36 ng/g	1/1		
	bottom ash	0.52 ng/g	1/1		

* x/y = detected in x of y samples
?: information unknown

Summary:

Studies on UV-320 are available from Sweden, Germany, Spain (and Portugal), USA, the Philippines, China and Japan. It has to be borne in mind that in Japan UV-320 is a Class I Specified Chemical Substance due to its PBT-properties since 2007 (Japan, 2007). This means that manufacture, import and use of UV-320 are prohibited in Japan. UV-320 has been detected in air, house and road dust, soil, surface water, sediments, aquatic organisms, WWTP influent, effluent and sludge, storm water, landfill effluent, combustible municipal solid waste and in flue gas, fly ash and bottom ash of a pilot scale waste incinerator.

Concentrations in air were below 1 ng/m³. In house and road dust few to several ng/g were measured (house dust max. 25 ng/g, road dust max. 3 ng/g).

Measured concentrations in surface water were below 1 ng/L. UV-320 was found in only one sample of wastewater (24 ng/L), WWTP effluent (4 ng/L) and storm water (< 1 ng/L), respectively. In landfill effluents measured concentrations were 7.3 and 23 ng/L.

Only one background soil sample from Sweden contained UV-320 (0.91 µg/g dw), whereas soil samples from Germany were free of the substance. Concentrations in sediments varied with concentrations of few µg/g dw in Sweden and some ng/g dw in Japan. Suspended solids from Germany did not contain UV-320. In WWTP sludge up to 2 µg/g dw were detected in Sweden, whereas no UV-320 was detected in China and Japan.

Concentrations in fish vary greatly. In the Swedish study the detection limit was high (0.9 µg/g dw) and no UV-320 was found. In the Philippines and in Japan concentrations up to several ng/g lw were detected (max. 74 ng/g lw). UV-320 is especially found in lipid of lower benthic organisms collected from tidal flat areas. In mussels up to 86 ng/g lw were detected. UV-320 also seems to be accumulated in the liver of some fish.

In combustible municipal solid waste UV-320 was present at a concentration of 7.1 ng/g. After combustion in a pilot-scale waste incinerator the flue gas still contained 2 ng/m³, the fly ash 0.36 ng/g and the bottom ash 0.52 ng/g.

CURRENT KNOWLEDGE ON ALTERNATIVES

Aside from the four Phenolic Benzotriazoles (UV-320, UV-327, UV-328, UV-350) for which Annex-XV-dossiers are currently presented there are further phenolic benzotriazoles which are also employed for the same uses, e.g. UV-P (CAS 2240-22-4), UV-326 (CAS. 3896-11-5), UV-234 (CAS 70321-86-7), UV-329 (CAS 3147-75-9), UV-360 (CAS 103597-45-1), UV-571 (CAS 125304-04-3), UV-928 (CAS 73936-91-1). With exception of UV-360 they differ only in the substitution pattern in the ortho- and para-position of the hydroxyl group. While the UV-absorption pattern is reported to be mainly not influenced by these substitutions there are effects on the solubility and the distinct coloration in different transparent plastic materials (Kirk et al., 2007). At least some of these substances appear to have similar PBT/vPvB-properties as the four substances currently in question and further work is currently done to assess these substances.

Besides the group of phenolic benzotriazoles there is also the group of benzophenones that are technically important UV-absorbers for transparent plastic materials. These substances are suspected to be potential endocrine disruptors.

Also, there is the group of Hindered Amine Light Stabilizers (HALS) that are technically important for the protection of plastic materials from UV-radiation. They do not work as UV-absorbents but as degradation inhibitors by being proton-donators. No information concerning the hazard assessment of this group was found.

RISK-RELATED INFORMATION

None.

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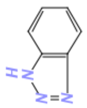
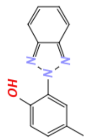
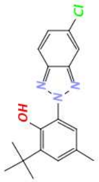
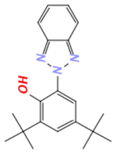
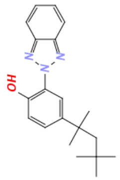
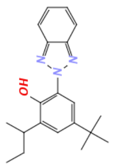
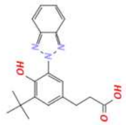
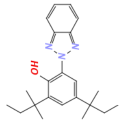
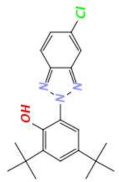
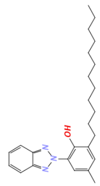
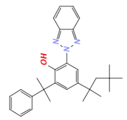
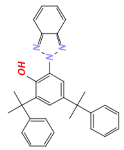
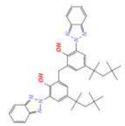
ANNEX 1: READ-ACROSS-DATA-MATRIX

In this matrix all available experimental results that might be relevant for the SVHC-identification are listed for all four substances in questions as well as all other substances mentioned in the dossier or used for a Read Across. The substances are ordered in order of rising molecular weight.

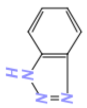
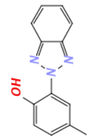
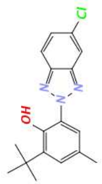
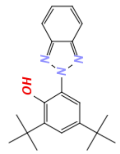
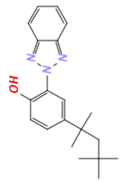
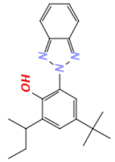
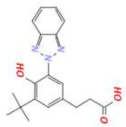
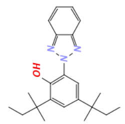
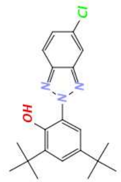
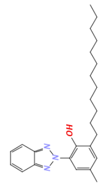
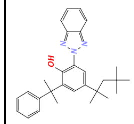
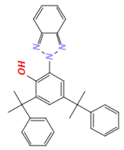
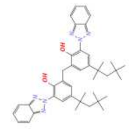
QSAR results were intentionally left out in this overview. In cases where several data points were available the most reliable one is presented and in cases where a decisions was not possible (as is for example the case for registration data disseminated on ECHAs webpage) all data point are presented.

Acronym	**1H-Benzotriazole**	**UV-P**	**UV-326**	**UV-320**	**UV-329**	**UV-350**	**M1**[6]	**UV-328**	**UV-327**	**UV-571**	**UV-928**	**UV-234**	**UV-360**
													
CAS No	95-14-7	2440-22-4	3896-11-5	3846-71-7	3147-75-9	36437-37-3	84268-36-0	25973-55-1	3864-99-1	125304-04-3	73936-91-1	70321-86-7	103597-45-1
EC No	202-394-1	219-470-5	223-445-4	223-346-6	221-573-5	253-037-1	-	247-384-8	223-383-8	-	422-600-5	274-570-6	403-800-1
Physicochemical Data													
Mol. Weight [g/mol]	119.1	225.3	315.8	323.4	323.4	323.4	339.4	351.5	357.9	393.6	441.6	447.6	658.9
log Kow	1.44[7]	4.31[7]										>6.5[8]	4.2[9]

[6] Degradation Product of EC 407-000-3

[7] Hansch, C. et al: Exploring QSAR Vol 2: Hydrophobic, Electronic, and Steric Constants (1995)

[8] The Phenolic Benzotriazoles Association: HPV Challenge Program, Data Summary and Test Plan for Phenoluic Benzotriazoles (2001)

Acronym	**1H-Benzotriazole**	**UV-P**	**UV-326**	**UV-320**	**UV-329**	**UV-350**	**M1**[6]	**UV-328**	**UV-327**	**UV-571**	**UV-928**	**UV-234**	**UV-360**
													
		4.2[8]											12.7[9,10]
pK_A	8.37[11]												
log Koc													5.63[9]
Water sol. [mg/L]	19800[12]	0.173[13]; 0.8[14]			<1[8]			0.015[14]	0.022[14]			<0.04 (at 20°)[8]	<0.007[9]
Vapor pressure [Pa]													$6\ 10^{-13}$ [9]
Data on Degradation													
ready biodegradability screening tests	non-biodegradable MITI-1 (OECD TG 301C),	Not readily biodegradable (OECD TG 301 B),		non-biodegradable MITI-1 (OECD TG 301C),	Not readily biodegradable (OECD TG 301 B),			Not readily biodegradable (OECD TG 301 B),	non-biodegradable MITI-1 (OECD TG 301C),		Not readily biodegradable (OECD TG 301 B),	Not readily biodegradable (OECD TG 301 B),	Biodegradation in water <10% (84/499/CEE method

9 Data disseminated on ECHA-Homepage

10 This value is so large that is probably not reliable

11 Serjeant,EP & Dempsey,B: Ionisation constants of organic acids in aqueous solution, p. 159 (1979)

12 Davis, LN et al: Investigation of selected potential environmental contaminants: benzotriazoles, USEPA-560/2-77-001 (1977)

13 US EPA Screening-LevelHazard Characterization Sponsored Chemicals Phenolic Benzotriazoles Category (2009)

14 Lopez-Avila, V & Hites, RA: EnvSciTechnol 11, p. 1382-1390 (1980)

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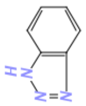
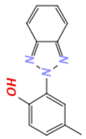
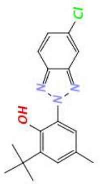
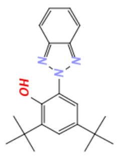
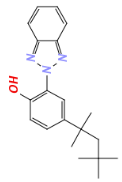
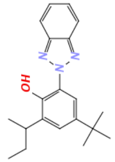
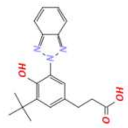
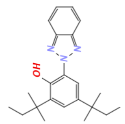
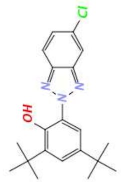
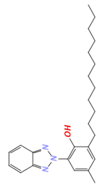
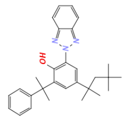
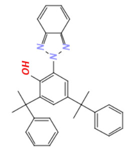
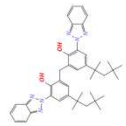
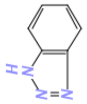
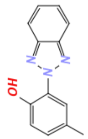
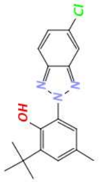
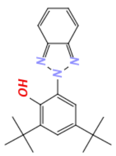
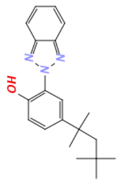
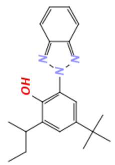
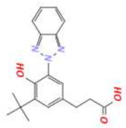
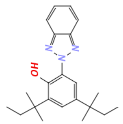
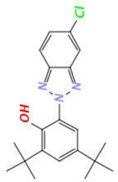
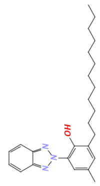
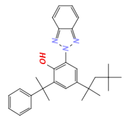
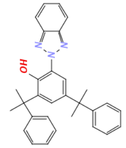
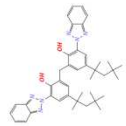
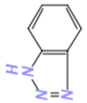
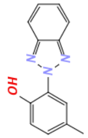
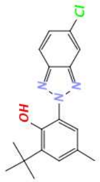
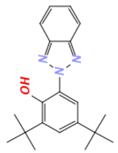
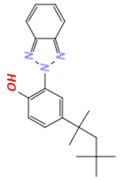
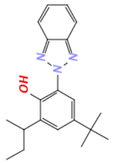
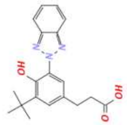
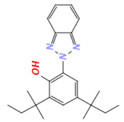
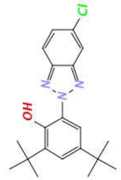
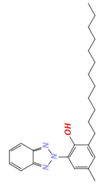
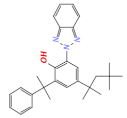
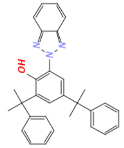
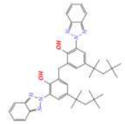
													
	BOD =2[15]	0–2% after 28 days[13]		BOD =0[15]	0–1% after 28 days[13]			2–8% after 28 days[13]	BOD =0[15]		-4–3% after 28 days[16]	3–8% after 28 days[13]	5)[9]; Biodegradation in water <2% (84/499/CEE method 5)[9]; Biodegradation in water 0% (84/499/CEE method 5)[9]
Simulation tests	Primary degradation aerobic: DT_{50}=114 d anaerobic:						OECD 308 aerobic: $DisT_{50}$ = 86 d (river system) $DisT_{11}$ =						

[15] Biodegradation and Bioconcentration Database of the Existing Chemical Substances; available: http://www.safe.nite.go.jp/jcheck/english/search.action

[16] Australia: Nantional Industrial Chemicals Notification and Assesment Scheme - Full Public Report - Tinuvin 928 (2000)

Acronym	**1H-Benzotriazole**	**UV-P**	**UV-326**	**UV-320**	**UV-329**	**UV-350**	**M1**[6]	**UV-328**	**UV-327**	**UV-571**	**UV-928**	**UV-234**	**UV-360**
													
	DT_{50}=144 d						44 d (pond system) anaerobic: build up until test was ended (100 d)						
Data on Bioaccumulation													
BCF (lipid normalized) acc. To OECD 305 C on Cyprinus carpio	1000 µg/L: 1-3; 100 µg/L: 5-17[15]	1000 µg/L: 171-686; 100 µg/L: 181-410; 10 µg/L: 55-275[15]	500 µg/L: 71-143; 50 µg/L: 258-1055; 5 µg/L: 721-1178[15]	10 µg/L: 1945; **1 µg/L: 5905; 0.1 µg/L: 12041**[15]		**1 µg/L: 20263; 0.1 µg/L: 34210**[15]		0.1 µg/L: 1121; 0.01 µg/L: 740-2148; **0.01 µg/L: 3681**[15]	1 µg/L: 1203; **0.1 µg/L: 6283/8817; 0.01 µg/L: 7540**[15]				
Field BAF calculat								**0.012 µg/L: 6429**[17]	**0.012 µg/L: 5946**[17]				

[17] : Nakata H et al.: Detection of benzotriazole UV stabilizers in the blubber of marine mammals by gas chromatography-high resolution mass spectrometry (GC-HRMS). J Environ Monit 12, p. 2088-2092 (2010)

Acronym	**1H-Benzotriazole**	**UV-P**	**UV-326**	**UV-320**	**UV-329**	**UV-350**	**M1**[6]	**UV-328**	**UV-327**	**UV-571**	**UV-928**	**UV-234**	**UV-360**
													
ed based on Nakata et al 2010 on Neophocaena phocaenoides													

ANNEX 2: OVERVIEW OF SELF-CLASSIFICATIONS

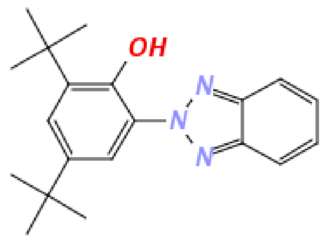
Table 19: Self Classification for UV-320 acc. to Regulation (EC) 1272/2008 (CLP)

Name / Tradename	EC-number	Hazard Class and Category Code(s)	Hazard Statement Code(s)
2-benzotriazol-2-yl-4,6-di-tert-butylphenol UV-320	223-346-6	Carc. 2 STOT RE 2 Aquatic Chronic 3	H351 H373 H412

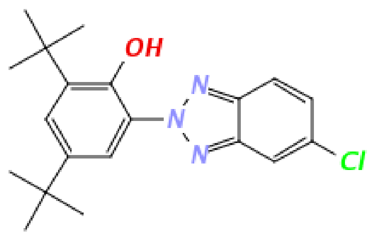
ANNEX 3: ANALYSIS OF QSAR APPLICATION: PREDICTION OF LOG KOC FOR UV-320, -327, -328 AND -350

A Information on substances and purpose

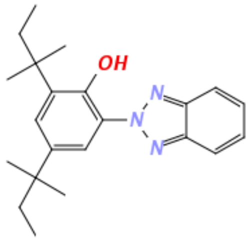
Molecule 1:

Name:	2-benzotriazol-2-yl-4,6-di-tert-butylphenol (UV-320)	
CAS Nr.	3846-71-7	
EU Nr.	223-346-6	
Smiles	c1(c(c(cc(c1)C(C)(C)C)C(C)(C)C)O)N(N=C2C=C3)N=C2C=C3	

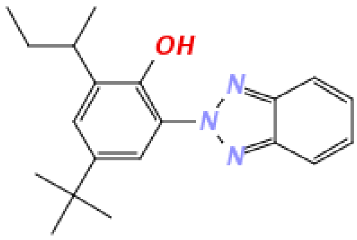
Molecule 2:

Name:	2,4-di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol (UV-327)	
CAS Nr.	3864-99-1	
EU Nr.	223-383-8	
Smiles	c1(c(c(cc(c1)C(C)(C)C)C(C)(C)C)O)N(N=C2C=C3)N=C2C=C3Cl	

Molecule 3:

Name:	2-(2H-benzotriazol-2-yl)-4,6-ditertpentylphenol (UV-328)	
CAS Nr.	25973-55-1	
EU Nr.	247-384-8	
Smiles	c1(c(c(cc(c1)C(C)(C)CC)C(C)(C)CC)O)N(N=C2C=C3)N=C2C=C3	

Molecule 4:

Name:	2-(2H-benzotriazol-2-yl)-4-(tert-butyl)-6-(sec-butyl)phenol (UV-350)	
CAS Nr.	36437-37-3	
EU Nr.	253-037-1	
Smiles	c1(c(c(cc(c1)C(C)(C)C)C(C)CC)O)N(N=C2C=C3)N=C2C=C3	

Endpoint	Logarithmic Partition coefficient of octanol-organic carbon
Regulatory purpose	PBT-Assessment, supporting information for a weight of evidence-approach to identify the substances as vP

B Relevant structure information

Parameter	Result	Rationale
Structure identification		
Structure of concern	parent	Substances are mono-constituents
Descriptors used for QSAR prediction		
Correction factors (KOCWIN KOW/MCI)	Applicable	All fragments are represented by the model
σ (COSMOtherm)	Applicable	The polarity was calculated on molecular structures geometrically optimized with Density-Functional-Theory (functional: Becke-Perdew 86, basis set of Triple-Zeta-Valence-Polarization-quality), all parameters for this method and all elements of the molecules are implemented
Other relevant information		
-	-	-

C QSAR models used

Model	Version	Endpoint	QMBI
(PC)KOCWIN - KOW method	V2.0	log K_{OC}	Annex 3.1
(PC)KOCWIN - MCI method	V2.0	log K_{OC}	Annex 3.2
COSMOtherm (K_{OC})	v. C30_1201	log K_{OC}	Annex 3.3

D Analysis of QSAR model performance

Model	QSAR result	Overall model performance	QPREF
KOCWIN KOW method	UV-320: 4.63	Reliable with restrictions	Annex 3.4
	UV-327: 4.99		
	UV-328: 5.18		
	UV-350: 4.66		
KOCWIN MCI method	UV-320: 5.07	Reliable with restrictions	Annex 3.4
	UV-327: 5.28		
	UV-328: 5.65		
	UV-350: 5.19		
COSMOtherm (K_{OC})	UV-320: 5.17	Reliable with restrictions	Annex 3.4
	UV-327: 5.64		
	UV-328: 5.46		
	UV-350: 4.90		

E Overall conclusion

Overall QSAR Result	Irrespective of the employed model all four substances have a high log K_{OC}. There does not seem to be a general systematic shift between the models and there is also no general order of the values when comparing the relative order of the results in the three models.
Rational	The log K_{OC} for all substances and all models is in the range of 4.63 to 5.65 log-units
Reliability	Reliable with restrictions.

Conclusion with regard to the regulatory purpose
The log K_{OC}-values for all four substances are high in all three models. The predictions are all in the same region, therefore these substances are similar in their behavior. According to the prediction the substances will bind strongly to sediment in the environment and therefore will mostly not be available for degradation processes.

ANNEX 3.1: QMBI KOCWIN KOW-method

	Information	**Literature references or Links**	**Remarks**
0 - General			
Model name and version	(PC)KOCWIN v.2 - KOW method	Online Help of KOCWIN	The KOCWIN – KOW method is essentially an extension of the MCI method were the descriptor MCI was replaced with K_{OW}. The same Trainings Sets and Validation Sets as for the MCI method were used and also the same Correction factors are applied. Overall the statistical performance of the KOW method is not quite as good as the MCI method.
W.a.[18]: software package	EPISUITE Estimation Programs Interface Suite™ for Microsoft® Windows, v4.10	http://www.epa.gov/oppt/exposure/pubs/episuite.htm	
1 - Definition of Endpoint			
Endpoint [units] (w.a. species and other relevant information)	Soil adsorption coefficient K_{OC} given as a logarithmic value		Defintion of K_{OC} according to Lyman et al, 1990: "the ratio of the amount of chemical adsorbed per unit weight of organic carbon (oc) in the soil or sediment to the concentration of the chemical in solution at equilibrium" Koc = (µg adsorbed/g organic carbon) / (µg/mL solution) [L/kg or mL/g]
2 – Definition of Algorithm			

[18] w.a.: when applicable

Brief description of algorithm and/or link to full definition	Non-polar chemicals (i.e. compounds where no correction factor is needed): $\log K_{oc} = 0.8679 \text{ Log } K_{ow} - 0.0004$ Polar chemicals (i.e. compounds where a correction factor is needed): $\log K_{oc} = 0.55313 \text{ Log } K_{ow} + 0.9251 + \Sigma P_f N$	See Online Help of KOCWIN	The equations were developed in a two separate regression calculations since this approach is statistically more accurate than the approach taken in the MCI-method
List of employed descriptors with units	Log KOW: logarithm of the n-octanol/water partition coefficient; P_f: correction factor for chemical class of functional group f; N: number of times chemical class or functional group f occurs	List of P_f available in Online Help of KOCWIN, Appendix D	
Number of Chemicals in Training Set and Brief description of it	Training Set comprises of non-polar set (68 chemicals) and a polar set (447 chemicals) taken from several literature sources. One compound of the original non-polar training set (hexabromobiphenyl) was not considered since there was no recommended experimental log K_{OW}.		Training Estimation Error: within <= 0.20 - 44.2% within <= 0.40 - 76.9% within <= 0.60 - 93.0% within <= 0.80 - 98.6% within <= 1.00 - 100% non-polar Training Set (n=68): r^2=0.877; std. dev.=0.478; avg. dev.= 0.371 polar Training Set (n=447): r^2=0.855; std. dev.=0.396; avg. dev.= 0.307
W.a.: Training set available at		Non-Polar Training Set: Online Help of KOCWIN, Appendix E Polar Set: Online Help of KOCWIN, Appendix F	

3 – Definition of the Applicability Domain			
W.a.: Definition of the Applicability Domain	Currently there is no universally accepted definition of model domain. Log Koc estimates are less accurate for compounds outside the MW range of the training set compounds and/or that have more instances of a given fragment than the maximum for all training set compounds. It is also possible that a compound may have a functional group(s) or other structural features not represented in the training set, and for which no fragment coefficient or correction factor was developed	List of correction factors available in Online Help of KOCWIN, Appendix D Non-Polar Training Set: Online Help of KOCWIN, Appendix E Polar Training Set: Online Help of KOCWIN, Appendix F	
Limits of the Applicability Domain	Molecular weight: 32.04-665.02 g/Mol Fragments and Functional groups according to Training Sets and correction factors for best results		
4 – Information on the Validation of the Model			
Validation Set Type	Internal, 150 compounds from the same sources as the Training Set. Eight ammonium and metal salt compounds were removed from the original Validation dataset of the MCI method. Compound Pool was split before regression into Training Set and Validation Set.		
W.a.: Validation available at		Online Help of KOCWIN, Appendix G	
Statistical information on validity	r^2=0.778; std. dev.=0.679; avg. dev.= 0.494		
5 – Mechanistic Interpretation of the model			
W.a.: Mechanistic basis of model	The tendency of a compound to adsorb itself on organic carbon is linked with its lipophilicity. The n-octanol/water partition coefficient is one descriptor for lipophilicity.		

ANNEX 3.2: QMBI KOCWIN MCI-method

	Information	Literature references or Links	Remarks
0 – General			
Model name and version	(PC)KOCWIN v.2 - MCI method	Meylan, W., P.H. Howard and R.S. Boethling, "Molecular Topology/Fragment Contribution Method for Predicting Soil Sorption Coefficients", *Environ. Sci. Technol*. 26: 1560-7 (1992)	Besides the MCI method there is also the KOW method implemented in KOCWIN. Overall the statistical performance of the MCI method is better than the KOW method.
W.a.[19]: software package	EPISUITE Estimation Programs Interface Suite™ for Microsoft® Windows, v4.10	http://www.epa.gov/oppt/exposure/pubs/episuite.htm	
1 - Definition of Endpoint			
Endpoint [units] (w.a. species and other relevant information)	Soil adsorption coefficient K_{OC} given as a logarithmic value		Defintion of K_{OC} according to Lyman et al, 1990: "the ratio of the amount of chemical adsorbed per unit weight of organic carbon (oc) in the soil or sediment to the concentration of the chemical in solution at equilibrium" Koc = (µg adsorbed/g organic carbon) / (µg/mL solution) [L/kg or mL/g]
2 – Definition of Algorithm			
Brief description of algorithm	log Koc = 0.5213 MCI + 0.60 + $\Sigma(P_f{*}N)$; MCI =	See Online Help of KOCWIN	MCI: Molecular Connectivity Index (in this case: First Order)

[19]w.a.: when applicable

and/or link to full definition	$\Sigma(\delta i*\delta j)^{-0.5}$		mathematical approach to describe molecular topology The equation was developed in a two step regression approach: 1. Derivation of equation without correction factors using a set of non polar chemicals 2. Derivation of final equation using a set of non-polar chemicals
List of employed descriptors with units	δi: δ-value of atom i, i.e. the number of adjacent non-hydrogen atoms; δj: δ–value of atom j, i.e. the number of adjacent non-hydrogen atoms; P_f: correction factor for chemical class of functional group f; N: number of times chemical class or functional group f occurs	List of P_f available in Online Help of KOCWIN, Appendix D	
Number of Chemicals in Training Set and Brief description of it	Training Set comprises of non-polar set (69 chemicals) and a polar set (447 chemicals) taken from several literature sources		Training Set Estimation Error: within <= 0.20 - 44.2% within <= 0.40 - 76.9% within <= 0.60 - 93.0% within <= 0.80 - 98.6% within <= 1.00 - 100% non-polar Training Set (n=69): r^2=0.967; std. dev.=0.247; avg. dev.= 0.199 polar Training Set (n=447):

			r^2=0.90; std. dev.=0.34; avg. dev.= 0.273
W.a.: Training set available at		Non-Polar Training Set: Online Help of KOCWIN, Appendix E Polar Set: Online Help of KOCWIN, Appendix F	
3 – Definition of the Applicability Domain			
W.a.: Definition of the Applicability Domain	Currently there is no universally accepted definition of model domain. Log Koc estimates are less accurate for compounds outside the MW range of the training set compounds and/or that have more instances of a given fragment than the maximum for all training set compounds. It is also possible that a compound may have a functional group(s) or other structural features not represented in the training set, and for which no fragment coefficient or correction factor was developed	List of correction factors available in Online Help of KOCWIN, Appendix D Non-Polar Training Set: Online Help of KOCWIN, Appendix E Polar Training Set: Online Help of KOCWIN, Appendix F	
Limits of the Applicability Domain	Molecular weight: 32.04-665.02 g/Mol Fragments and Functional groups according to Training Sets and correction factors for best results		
4 – Information on the Validation of the Model			
Validation Set Type	Internal, 158 compounds from the same sources as the Training Set. Compound Pool was split before regression into Training Set and Validation Set.		
W.a.: Validation available at		Online Help of KOCWIN, Appendix G	
Statistical information on validity	r^2=0.850; std. dev.=0.583; avg. dev.= 0.459		
5 – Mechanistic Interpretation of the model			

W.a.: Mechanistic basis of model	The tendency of a compound to adsorb itself on organic carbon is linked with the chemical structure. In the Molecular Correction Index information on the chemical structure, i.e. molecular size, branching, cyclization, unsaturation and (to a certain extent) heteroatom content are encoded. The different influences of chemical classes or functional groups are considered by correction factors.		

ANNEX 3.3: QMBI COSMOtherm (K_{OC})

	Information	**Literature references or Links**	**Remarks**
0 - General			
Model name and version	COSMOtherm v C30_1201		The COSMOtherm model allows in principle the calculation of all partition properties of molecules. In this QMBI only the calculation of the K_{OC} will be addressed
W.a.[20]: software package	COSMOtherm		
1 - Definition of Endpoint			
Endpoint [units] (w.a. species and other relevant information)	n-octanol/organic carbon partition coefficient given as a logarithmic value		
2 – Definition of Algorithm			
Brief description of algorithm and/or link to full definition	$\text{Log } K_{OC} = 0.0168 \cdot M_0^X - 0.017 \cdot M_2^X - 0.040 \cdot M_3^X + 0.19 \cdot PM_{acc}^X - 0.27 \cdot M_{don}^X + 0.37$ with $M_i^X = \int p^X \sigma^i d\sigma$ for i = 0, 2, 3. $M_{acc}^X = 0$ if $\sigma < 1$ e/nm^2 or $= \sigma - 1$ e/nm^2 if $\sigma > 1$ e/nm^2 and $M_{don}^X = 0$ if $-\sigma < 1$ e/nm^2 or $= -\sigma - 1$ e/nm^2 if $-\sigma > 1$ e/nm^2	"COSMO-RS: From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design", Andreas Klamt, Elsevier Science Ltd., Amsterdam, The Netherlands (2005), ISBN: 0-444-51994-7. "Prediction Of Soil Sorption Coefficients With A Conductor-Like Screening Model For Real Solvents", Andreas Klamt, Frank	COSMOtherm implements the COSMO-RS theory. This theory interprets the interaction of molecules as an interaction of a larger ensemble of molecular surfaces calculated with Quantum Mechanical methods. Due to a treatment with statistical thermodynamics the macroscopic properties of interacting molecules like partition coefficients become available. If the partition is with a phase that is ill defined like organic carbon, the so called σ-moment approach is employed where a solvent is represented as a linear combination of six σ-functions. The coefficients to these functions are fitted with

[20] w.a.: when applicable

		Eckert and Michael Diedenhofen, *Environmental Toxicology and Chemistry*, **21**, 2562-2566 (2002).	experimental data.
List of employed descriptors with units	σ: Screening charge density or polarity, i.e. the electrostatic screening of a solute molecule by its surrounding and its back polarization in a region with radius of ca. 0.5 Å ; p^X: sigma profile of molecule X, i.e. the sum of the probability distributions of all possible σ		
Number of Chemicals in Training Set and brief description of it	Original parameterization for COSMOtherm: 225 small- and medium-sized organic compounds with H, C, O, N, Cl atoms. The fitting was done for 650 experimental room-temperature parameters (ΔG_{hydr}, log(vapor pressure), log $K_{octanol-water}$, log $K_{hexane-water}$, log $K_{benzene-water}$, log $K_{diethyl\ ether-water}$ log K_{OC}-formula: 387 molecules (performance: r^2 = 0.72, rms = 0.62 log-units)		While the principle theory is applicable for all elements, the practical implementation needs some specific parameters to the QM-method used and the elements of the substance in question like the employed ratio for scaling the bonds of the QM-method and the van der Waals-coefficients
W.a.: Training set available at		Original parameterization for COSMOtherm: "Refinement and Parametrization of COSMO-RS", Andreas Klamt, Volker Jonas, Thorsten Bürger and John C. W. Lohrenz, *J. Phys. Chem. A* **102**, 5074-5085 (1998). Log K_{OC}-formula: "Prediction Of Soil Sorption Coefficients With A Conductor-Like Screening Model For Real Solvents", Andreas Klamt, Frank Eckert and Michael Diedenhofen, *Environmental Toxicology and Chemistry*, **21**, 2562-2566 (2002).	Original parameterization for COSMOtherm: Since the original parameterization was done further adjustments were made and parameters for further elements were introduced. While the parameters are available in the software, to our knowledge the details of the new parameterisations were not disclosed

3 – Definition of the Applicability Domain			
W.a.: Definition of the Applicability Domain	There is no formal definition of the applicability domain		
Limits of the Applicability Domain	In principle the method is completely based on first-principles meaning there is no limit of the Applicability Domain.		
4 – Information on the Validation of the Model			
Validation Set Type	The KOC-model was tested against 53 demanding chemicals achieving a rmd of 0.72		
W.a.: Validation available at		"Prediction Of Soil Sorption Coefficients With A Conductor-Like Screening Model For Real Solvents", Andreas Klamt, Frank Eckert and Michael Diedenhofen, *Environmental Toxicology and Chemistry*, **21**, 2562-2566 (2002).	
Statistical information on validity	-		
5 – Mechanistic Interpretation of the model			
W.a.: Mechanistic basis of model	The interaction of a solute and a solvent is calculated in terms of a chemical potential. The difference of the chemical potentials of the solute in two different solvents is the mechanistic reason for partition effects.		

ANNEX 3.4: Analysis of QSAR prediction for UV-320 , UV-327, UV-328, UV-350

QSAR Model: KOCWIN KOW-method, KOCWIN MCI-method and COSMOtherm (K_{OC})

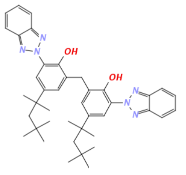
Overall performance

	Result		Further description
Endpoint results [unit]	KOCWIN KOW-method	UV-320: 4.63	All log KOC-values are high and in a similar region.
		UV-327: 4.99	
		UV-328: 5.18	
		UV-350: 4.66	
	KOCWIN MCI-method	UV-320: 5.07	
		UV-327: 5.28	
		UV-328: 5.65	
		UV-350: 5.19	
	COSMOtherm (K_{OC})	UV-320: 5.17	
		UV-327: 5.64	
		UV-328: 5.46	
		UV-350: 4.90	
Applicability domain	Yes		The molecules are in the range of all descriptors employed in the models.
Similarity with trainings set	Yes		All fragments or elements of the molecules are represented in the Training Set of KOCWIN. COSMOtherm has no training set but is generally applicable.
Similar substances	One		See table next side, substance is not very similar
Model performance for similar substances	Mediocre		There is just one experimental value of unknown quality for a substance not very similar to the substances at hand. The prediction for this substance is much higher than the experimental value but both values are high.
Other uncertainties	No		-

Overall conclusion	Reliable

Rational	As the models are applicable and results for similar molecules and two of the four models at hand show values in the same range it can be expected that the range is correctly predicted.

Results for similar substances

	Substance 1
Structure	
CAS-Nr.	103597-45-1
EU-Nr.	403-800-1
(Trade-)Name	UV-360
Descriptor value	KOCWIN KOW-method : log K_{OC} = 11.08 KOCWIN KOW-method : log K_{OC} = 8.22 COSMOtherm: log K_{OW} = 7.91
Predicted endpoint	See above
Experimental endpoint	5.63
Statistical performance	-

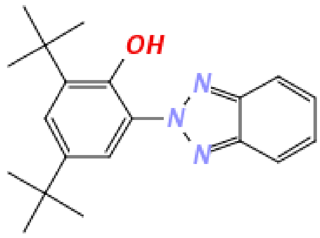
Rationale for the selection of similar substances

Substance 1 is a phenolic benzotriazole as the target molecule but it is a molecule comprised of two phenolic benzotriazole bodies therefore the similarity is not very high. Since the functional groups are nevertheless the same and since there are no other phenolic benzotriazoles were a experimental log K_{OC} is reported, UV-360 was chosen as point of reference.

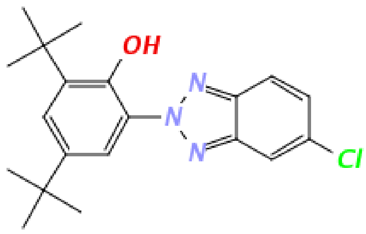
ANNEX 4: ANALYSIS OF QSAR APPLICATION: PREDICTION OF LOG KOW FOR UV-320, -327, -328 AND -350

A Information on substances and purpose

Molecule 1:

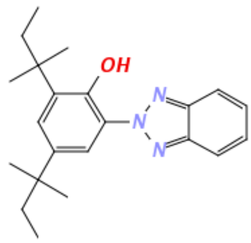
Name:	2-benzotriazol-2-yl-4,6-di-tert-butylphenol (UV-320)	
CAS Nr.	3846-71-7	
EU Nr.	223-346-6	
Smiles	c1(c(c(cc(c1)C(C)(C)C)C(C)(C)C)O)N(N=C2C=C3)N =C2C=C3	

Molecule 2:

Name:	2,4-di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol (UV-327)	
CAS Nr.	3864-99-1	
EU Nr.	223-383-8	
Smiles	c1(c(c(cc(c1)C(C)(C)C)C(C)(C)C)O)N(N=C2C=C3)N =C2C=C3Cl	

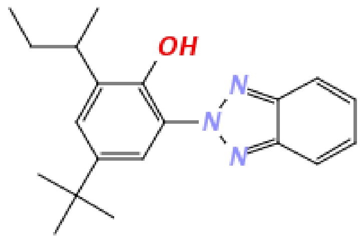
Molecule 3:

Name:	2-(2H-benzotriazol-2-yl)-4,6-ditertpentylphenol (UV-328)
CAS Nr.	25973-55-1
EU Nr.	247-384-8
Smiles	c1(c(c(cc(c1)C(C)(C)CC)C(C)(C)CC)O)N(N=C2C=C3)N=C2C=C3



Molecule 4:

Name:	2-(2H-benzotriazol-2-yl)-4-(tert-butyl)-6-(sec-butyl)phenol (UV-350)
CAS Nr.	36437-37-3
EU Nr.	253-037-1
Smiles	c1(c(c(cc(c1)C(C)(C)C)C(C)CC)O)N(N=C2C=C3)N=C2C=C3



Endpoint	Logarithmic Partition coefficient of octanol-water
Regulatory purpose	PBT-Assessment, supporting information

B Relevant structure information

Parameter	Result	Rationale
Structure identification		
Structure of concern	parent	Substances are mono-constituents
Descriptors used for QSAR prediction		
Fragment descriptors (KOWWIN)	applicable	All fragments are represented by the model
σ (COSMOtherm)	applicable	The polarity was calculated on molecular structures geometrically optimized with employing Density-Functional-Theory (functional: Becke-Perdew 86, basis set of Triple-Zeta-Valence-Polarization-quality), all parameters for this method and all elements of the molecules are implemented
Other relevant information		
-	-	-

C QSAR models used

Model	Version	Endpoint	QMBI
KOWWIN	v1.68	log K_{OW}	Annex 4.1
COSMOtherm (K_{OW})	v. C30_1201	log K_{OW}	Annex 4.2

D Analysis of QSAR model performance

Model	QSAR result	Overall model performance	QPREF
KOWWIN	UV-320: 6.27	Reliable	Annex 4.3
	UV-327: 6.91		
	UV-328: 7.25		
	UV-350: 6.31		
COSMOtherm (K_{OW})	UV-320: 7.39	Reliable	Annex 4.3
	UV-327: 7.91		
	UV-328: 7.89		
	UV-350: 7.11		

E Overall conclusion

Overall QSAR Result	All four substances have a very high log K_{OW} that is above the screening criterion for bioaccumulation in the PBT-assessment. The substances behave similar. Also KOWWIN predicts log KOWs approximately 0.8-1.0 log units smaller than COSMOtherm. The values of KOWWIN are nearer to the available experimental values.
Rationale	Not B-Screening criteria according to ECHA Guidance R.11 is log K_{OW} < 4.5
Reliability	Reliable

Conclusion with regard to the regulatory purpose
The log K_{OW}-values for all four substances are high and therefore a high bioaccumulation potential is expected. This expectation is confirmed by the available experimental BCF-values. All four substances have log K_{OW}-values in the same region. While there seems to be a systematic shift between the results there is no such shift observed for the relative order of the values.

ANNEX 4.1: QMBI KOWWIN

	Information	Literature references or Links	Remarks
0 - General			
Model name and version	KOWWIN 1.68	Meylan, W.M. and P.H. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84: 83-92.	
W.a.[21]: software package	EPISUITE Estimation Programs Interface Suite™ for Microsoft® Windows, v4.10	http://www.epa.gov/oppt/exposure/pubs/episuite.htm	
1 - Definition of Endpoint			
Endpoint [units] (w.a. species and other relevant information)	n-octanol/water partition coefficient given as a logarithmic value		
2 – Definition of Algorithm			
Brief description of algorithm and/or link to full definition	$\text{Log } K_{OW} = \Sigma(f_i{*}n_i) + \Sigma(c_j{*}n_j) + 0.229$	See Online help of KOWWIN	Derived by multiple regression of training set in a two step procedure: 1. Derivation of f_i 2. Introduction of c_j
List of employed descriptors with units	f_i: coefficient for each atom or fragment i; n_i: number of times fragment/atom i occurs; c_j: coefficient for correction instance j; number of times a structure that leads to a correction instance occurs	See Online help of KOWWIN, Appendix D	There are 157 different atoms and fragments defined and 278 correction factors that are employed when certain chemical classes or functional groups are present in the molecule for which an estimation is made

[21]w.a.: when applicable

Number of Chemicals in Training Set and Brief description of it	2447 chemicals with measured log K_{OW}-values from the PhysProp Database		Training Set Estimation Error: within <= 0.10 - 45.0% within <= 0.20 - 72.5% within <= 0.40 - 92.4% within <= 0.50 - 96.4% within <= 0.60 - 98.2%
W.a.: Training set available at		List available at http://esc.syrres.com/interkow/KowwinData.htm	
3 – Definition of the Applicability Domain			
W.a.: Definition of the Applicability Domain	Currently there is no universally accepted Applicability Domain, but in principle by molecular weight range and by fragments and their maximum occurrence, both defined by the Training Set; while also substances with specific behavior in liquids like dissociation or surfactant-specific properties were included, these are not explicitly considered in the model		With exceedingly high or low log K_{OW} the experimental errors for determination of log K_{OW} will become larger and therefore the uncertainty. In such cases the predicted values will be more uncertain as well.
Limits of the Applicability Domain	18.02 to 719.92 [g/Mol], for Structural Domain see Training Set		
4 – Information on the Validation of the Model			
Validation Set Type	Approximately 10.946 chemicals from different sources		
W.a.: Validation available at		List available at http://esc.syrres.com/interkow/KowwinData.htm	
Statistical information on validity	Validation Set Estimation Error: within <= 0.20 - 39.6%		Details available in Online help of KOWWIN

	within <= 0.40 - 66.0% within <= 0.50 - 75.6% within <= 0.60 - 82.5% within <= 0.80 - 91.6% within <= 1.00 - 95.6% within <= 1.20 - 97.7% within <= 1.50 - 99.1%		
5 – Mechanistic Interpretation of the model			
W.a.: Mechanistic basis of model	Fragment coefficients and correction factors reflect the impact of certain chemical fragments or functional groups on lipophilicity and thus on the log K_{OW}.		

ANNEX 4.2: QMBI COSMOtherm KOW

	Information	**Literature references or Links**	**Remarks**
0 - General			
Model name and version	COSMOtherm v C30_1201		The COSMOtherm model allows in principle the calculation of all partition properties of molecules. In this QMBI only the calculation of the K_{OW} will be addressed
W.a.[22]: software package	COSMOtherm		
1 - Definition of Endpoint			
Endpoint [units] (w.a. species and other relevant information)	n-octanol/water partition coefficient given as a logarithmic value		
2 – Definition of Algorithm			
Brief description of algorithm and/or link to full definition	$\log K_{OW}(T) = \int p^i(\sigma)(\mu_{water}(\sigma;T) - \mu_{octanol}(\sigma;T))d\sigma + \mu_i^C(\text{water}, T) - \mu_i^C(\text{octanol},; T)$, where $\mu_i^C(S, T) = RT^* [\lambda_0^* \ln r_i + \lambda_1^*(1-(r_i/\underline{r} - \ln \underline{r}) + \lambda_2^*(1-q_i/\underline{q} - \ln \underline{q})]$ and $\underline{r} = \Sigma_I x_i^* r_i$ and $\underline{q} = \Sigma_i x_i^* q_i$	"COSMO-RS: From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design", Andreas Klamt, Elsevier Science Ltd., Amsterdam, The Netherlands (2005), ISBN: 0-444-51994-7.	COSMOtherm implements the COSMO-RS theory. This theory interprets the interaction of molecules as an interaction of a larger ensemble of molecular surfaces calculated with Quantum Mechanical methods. Due to a treatment with statistical thermodynamics the macroscopic properties of interacting

[22] w.a.: when applicable

			molecules like partition coefficients become available.
List of employed descriptors with units	R: Ideal gas constant [kcal/(mol K)], T: temperature [K]; σ: Screening charge density or polarity, i.e. the electrostatic screening of a solute molecule by its surrounding and its back polarization in a region with radius of ca. 0.5 Å ; $p^i(\sigma)$: sigma profile of molecule i, i.e. the sum of the probability distributions of all possible σ; $\mu_{water}(\sigma;T)$: sigma potential of water at temperature T, a sigma potential can be interpreted as the affinity of a molecule for a surface of polarity σ; $\mu_{octanol}(\sigma;T)$: sigma potential of octanol at temperature T; $\mu_i^C(S;T)$: combinatorial contribution to the chemical potential of molecule i in solvent S at temperature T; λ_0, λ_1, λ_2: adjustable parameters, r_i: molecular volume of substance i, q_i: molecular area of substance i, $\underline{r}$: overall volume of the mixture, $\underline{q}$: overall area of the mixture.		
Number of Chemicals in Training Set and brief description of it	Original parameterisation: 225 small- and medium-sized organic compounds with H, C, O, N, Cl atoms. The fitting was done for 650 experimental room-temperature parameters (ΔG_{hydr}, log(vapor pressure), log $K_{octanol-water}$, log $K_{hexane-water}$, log $K_{benzene-water}$, log $K_{diethyl\ ether-water}$		While the principle theory is applicable for all elements, the practical implementation needs some specific parameters to the QM-method used and the elements of the substance in question like the employed ratio for scaling the bonds of the QM-method and the van der Waals-coefficients
W.a.: Training set available at		"Refinement and Parametrization of COSMO-RS", Andreas Klamt, Volker Jonas, Thorsten Bürger and John C. W. Lohrenz, *J. Phys. Chem. A* **102**, 5074-5085 (1998).	Since the original parameterization was done further adjustments were made and parameters for further elements were introduced. While the parameters are available in the software, to our knowledge the details of the new

			parameterisations were not disclosed
3 – Definition of the Applicability Domain			
W.a.: Definition of the Applicability Domain	There is no formal definition of the applicability domain		
Limits of the Applicability Domain	In principle the method is completely based on first-principles meaning there is no limit of the Applicability Domain.		
4 – Information on the Validation of the Model			
Validation Set Type	To our knowledge there is no single validation set but there are several citations in literature on the accuracy/validity of the model		
W.a.: Validation available at		Overview over publications: http://www.cosmologic.de/index.php?cosId=4150&crId=10	
Statistical information on validity	-		
5 – Mechanistic Interpretation of the model			
W.a.: Mechanistic basis of model	The interaction of a solute and a solvent is calculated in terms of a chemical potential. The difference of the chemical potentials of the solute in two different solvents is the mechanistic reason for partition effects.		

ANNEX 4.3: Analysis of QSAR prediction for UV-320 , UV-327, UV-328, UV-350

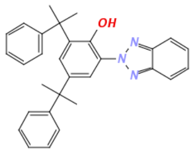
QSAR Model: KOWWIN and COSMOtherm (K_{OW})

Overall performance

	Result		Further description
Endpoint results [unit]	KOWWIN	UV-320: 6.27	All log KOW-values are high and in a similar region. There seems to be a systematic shift between the two models where KOWWIN predicts in general lower values.
		UV-327: 6.91	
		UV-328: 7.25	
		UV-350: 6.31	
	COSMO-therm (K_{OW})	UV-320: 7.39	
		UV-327: 7.91	
		UV-328: 7.89	
		UV-350: 7.11	
Applicability domain	Yes		The molecules are in the range of all descriptors employed in the models and in the range of the molecular weight of the molecules in the training set of KOWWIN.
Similarity with trainings set	Yes		All fragments or elements of the molecules are represented in the Training Set of KOWWIN. COSMOtherm has no training set but is generally applicable.
Similar substances	Yes		See table next side
Model performance for similar substances	Concerning the range of values good, but absolute values seem to be slightly overestimated		Experimental Values and predictions show a systematic shift but caution has to be advised as the experimental values were not validated.
Other uncertainties	No		-

Overall conclusion	Reliable
Rational	As the models are applicable and results for similar molecules and two of the four models at hand show values in the same range it can be expected that the range is correctly predicted.

Results for similar substances

	Substance 1
Structure	
CAS-Nr.	70321-86-7
EU-Nr.	274-570-6
(Trade-)Name	UV-234
Descriptor value	KOWWIN : log K_{OW} = 7.67 COSMOtherm: log K_{OW} = 8.30
Predicted endpoint	See above
Experimental endpoint	> 6.5
Statistical performance	-

Rationale for the selection of similar substances

Substance 1 is structurally similar as it is a phenolic benzotriazole as the target molecule. It also has a sterical demanding side chain in ortho- and one in para-position to the hydroxyl group. The difference lies in the substitution of a phenyl group for a methyl group. Therefore is is probably to some degree more lipophilic as UV-327.

ANNEX 5 MONITORING OF PHENOLIC BENZOTRIAZOLES

Monitoring studies are summarized concerning the following phenolic benzotriazoles:

UV-234 (CAS 70-321-86-7), -320 (CAS 3846-71-7), -326 (CAS 3896-11-5), -327 (CAS 3864-99-1), -328 (CAS 25973-55-1), -329 (CAS 3147-75-9), -350 (CAS 36437-37-3), -360 (CAS 103597-45-1) and -571 (CAS 125304-04-3). No monitoring studies were found for UV-928 (CAS 73936-91-1).

European studies:

Brorström-Lundén et al. (Brorström-Lundén et al., 2011) published a screening study on benzotriazoles (UV-234, -320, -327, -328, -329, -360). Phenolic benzotriazoles may to a large extent enter Sweden through imported finished goods. Emissions via diffuse sources were assumed as the main pathway of benzotriazole UV-absorbers to the environment. The sampling program was therefore focused on emissions in urban environments (Stockholm area and smaller city Borås). In addition background sites were included and two sites with potential point sources. Benzotriazoles were analyzed using an LC-MS system including a tandem mass-spectrometer. Detection limits vary with analyzed substance and sample. Compared to other studies the detection limits for sediment, soil, particles, WWTP sludge and fish are high.

Table 20: Detection limits in the investigation of Brorström-Lundén et al.

Compartment	Detection limits	Compartment	Detection limits
Air	0.01 – 0.48 ng/m³	storm water	0.03 – 0.1 ng/L
air deposition	30 – 200 ng/m² day	landfill effluent particles	0.7 -1.6 µg/g dw
surface water	0.03 – 0.09 ng/L	landfill effluent	0.08 – 0.5 ng/L
Sediment	0.2 – 12 µg/g dw	WWTP effluent particles	61 – 130 µg/g dw
Soil	0.1 – 0.9 µg/g dw	WWTP effluent	0.04 – 0.1 ng/L
Fish	0.3 – 1.9 µg/g dw	sludge	0.1 – 0.6 µg/g dw

In air samples 4 benzotriazole UV-absorbers were detected (UV-320, -327, -329, -360). Concentrations were similar in background and urban air. However, the highest concentration was measured in Stockholm. Only two compounds were detected in atmospheric deposition (UV-327, -329). The deposition was higher at the urban site.

Table 21: Concentrations of phenolic benzotriazoles in air and atmospheric deposition in Sweden

Substance	Air		Deposition	
	detected in x of y	concentration	detected in x of y	deposition flux

	samples [x/y]	[ng/m³]	samples [x/y]	[ng/m² day]
UV-234	0/8	-	0/4	-
UV-320	3/8	0.024 – 0.67	0/4	-
UV-327	6/8	0.40 - 25	3/4	<100-320
UV-328	0/8	-	0/4	-
UV-329	5/8	< 0.15 – 3.0	3/4	<100-331
UV-360	1/8	0.40	0/4	-

Several benzotriazoles were found in soil, in rather similar concentrations at the background and the urban locations (UV-320, -327, -328, -329). There were differences in the occurrence among the individual substances at the different locations. According to the authors the highest concentration of a single substance (UV-329) was found in Soil 500 m from a busy road in the Stockholm area. However, according to the annex of the study such a high concentration was also found for UV-327 in another urban sample. Since only 4 samples were analyzed altogether, the results should generally be interpreted with care.

Several of the benzotriazoles were frequently detected in surface water (UV-320, -327, -328. -329). The concentrations were mostly similar at background and urban locations. In sediments the distribution among different substances varied for the different sampling sites. Peaks of single substances occurred both at background and urban locations; the lower concentration levels were similar at different locations.

Three of the benzotriazoles were found in fish, both at urban and background locations (UV-324, -327, -329). The highest concentration was found at the background location (UV-327). The concentrations found in Swedish fish are 1000fold higher than those found in Japanese fish. The reason for this is unknown. The authors note however that most substances are not detected and the levels found are quite close to the detection limit of the method used.

Table 22: Concentrations of phenolic benzotriazoles in soil and fish in Sweden

Substance	**Soil**		**Fish**	
	detected in x of y samples [x/y]	concentration [µg/g dw]	detected in x of y samples [x/y]	concentration [µg/g dw]
UV-234	0/4	-	1/4	0.26
UV-320	1/4	0.91	0/4	-
UV-327	3/4	0.66-3.7	3/4	2.3-9.8
UV-328	1/4	0.74	0/4	-
UV-329	3/4	0.79-3.7	3/4	1-2.5
UV-360	0/4	-	0/4	-

Table 23: Concentrations of phenolic benzotriazoles in surface water and sediment in Sweden

Substance	Surface water		sediment	
	detected in x of y samples [x/y]	concentration [ng/L]	detected in x of y samples [x/y]	concentration [µg/g dw]
UV-234	0/6	-	0/6	-
UV-320	3/6	0.55-0.94	5/6	0.16-3
UV-327	4/6	0.11-0.39	6/6	1.6-35
UV-328	6/6	1.3-10	4/6	0.65-1.3
UV-329	6/6	0.25-2.4	4/6	0.81-33
UV-360	1/6	0.16	3/6	0.42-2.9

All benzotriazoles but UV-360 were detected in WWTP effluent and all substances were detected in sludge from WWTPs. However, there were differences both in concentration levels and in distribution among the different benzotriazoles between the WWTPs. A different distribution among the substances was also found in effluent and sludge. Only one sample of WWTP effluent particles was analyzed and only UV-327 was detected in this sample (270 µg/g dw).

Table 24: Concentrations of phenolic benzotriazoles in WWTP effluent and sludge in Sweden

Substance	effluent WWTP		sludge WWTP	
	detected in x of y samples [x/y]	concentration [ng/L]	detected in x of y samples [x/y]	concentration [µg/g dw]
UV-234	1/5	0.11	8/8	2.1-7.3
UV-320	1/5	4	6/8	0.84-2
UV-327	4/5	0.12-0.48	7/8	0.54-17
UV328	5/5	6.8-15	4/8	2.8-37
UV-329	5/5	0.87-4.9	7/8	2.3-15
UV-360	0/5	-	8/8	4.6-23

All substances but UV-360 were found in landfill leachates, all substances but UV-329 occurred in storm water. In one sample of landfill effluent particles UV-327, -328 and -329 were detected in concentrations of 4.3, 3.1 and 6.1 µg/g dw, respectively.

Table 25: Concentrations of phenolic benzotriazoles in effluent landfill and storm water in Sweden

Substance	effluent landfill		storm water	
	detected in x of y samples [x/y]	concentration [ng/L]	detected in x of y samples [x/y]	concentration [ng/L]
UV-234	2/3	0.16 and 0.5	4/4	0.06-0.31

UV-320	2/3	7.3 and 23	1/4	0.73
UV-327	2/3	0.45 and 1.3	3/4	0.13-0.17
UV-328	3/3	7-91	3/4	0.19-1.3
UV-329	1/3	17	0/4	-
UV-360	0/3	-	2/4	0.17 and 0.28

In summary widespread occurrence of benzotriazoles in the Swedish environment was observed both in background and urban areas. The substances occurred in all environmental matrices included in the study: air, deposition, surface water, sediment, soil and biota. Diffuse spreading through WWTPs, landfills and storm water may be important for the occurrence in the environment. Levels measured in WWTP effluents and sludge indicate widespread diffusive sources via use of products. The benzotriazoles with the highest usage volume in Sweden (UV-327, UV-328) were also most often found in the highest concentrations.

The authors conclude that on a national scale air transport may be a significant source of the compounds and that the substances are stable enough to undergo atmospheric long range transport.

Carpinteiro et al. (Carpinteiro et al., 2010a) used headspace solid-phase microextraction followed by gas chromatography tandem mass spectrometry for the sensitive determination of benzotriazole UV-stabilizers in water samples (UV-326, -327, -328). The limit of quantification was < 2 ng/l. The developed methodology was used to investigate the presence of benzotriazoles in filtered river water (3 samples), two samples taken in the inlet and outlet streams of an urban WWTP and four additional specimens of raw wastewater provided by a local laboratory. Phenolic benzotriazoles were not detected in river water and treated wastewater. In raw wastewater samples UV-327 was not detected, whereas UV-326 and -328 were each found in 4 of 5 samples in concentrations ranging from 3.5-57 ng/L and 1-19 ng/L, respectively.

Carpinteiro et al. (Carpinteiro et al., 2010b) also investigated benzotriazole UV-stabilizers in indoor dust samples (UV-326, -327 and -328). Pressurized liquid extraction and gas chromatography followed by tandem in time mass spectrometry were used. The limits of quantification were between 4 and 9 ng/g. Procedural blanks showed small peaks at the retention time of some species. The source of this contamination may be related to the trend of target compounds to be retained on solid surfaces. Glass material, extraction cells and connections in the extraction system might contribute to the presence of benzotriazole UV-stabilizers in procedural blanks due to carry over problems.

Dust was collected with domestic vacuum cleaners equipped with paper filter bags from several private houses (5 samples), vehicle cabins (3 samples) and an administrative building (1 sample). It is not stated in which country the dust was collected. However, we assume that it was collected in Spain. The dust fraction < 60 µm was used for the study. In addition a house dust reference material from USA was acquired. This sample was used to confirm the ubiquity of benzotriazole UV-stabilizers in dust although no certified or indicative values of their levels in the reference material were available.

UV-326, -327 and -328 were found to be ubiquitous in dust, with measured values from 22 to >600 ng/g. Moreover, UV-326 was found in one car cabin dust sample at a concentration of almost 5 µg/g.

Table 26: Levels of benzotriazole light stabilizers in dust samples (n = 3 replicates) [ng/g]

	UV-326	**UV-327**	**UV-328**
private house 1	42	86	46
private house 2	58	101	127
private house 3	333	29	100
private house 4	73	22	68
private house 5	269	52	149
public building	676	131	62
car cabin 1	4880	48	88
car cabin 2	522	127	124
car cabin 3	170	43	52
US dust reference material	121	322	259
Min-Max (Mean) of all samples except US material	42 – 4883 (780)	22 – 127 (71)	46 – 149 (91)

Carpinteiro et al. (Carpinteiro et al., 2012b) combined stir-bar sorptive extraction and liquid desorption with large volume injection-gas chromatography-mass spectrometry for the determination of benzotriazole UV-stabilizers in wastewater matrices. UV-320, -326, -327 and -328 were measured in urban sewage waters. Grab samples of wastewater were obtained from inlet and outlet streams of two urban WWTPs, equipped with primary and activated sludge treatment units, located in Portugal and Spain. The limits of quantification were between 4 and 10 ng/L. Because of the existence of significant concentrations of phenolic benzotriazoles associated with dust particles it is highly recommended to protect laboratory material from deposition of particulate matter. The efficiency of the extraction is sample dependent; therefore, the standard addition method is required for the accurate quantification of the substances in wastewater matrices.

Table 27: Average concentrations of phenolic benzotriazoles in wastewater matrices (n = 3 replicates) [ng/L]

Place, date	type	UV-320	UV-326	UV-327	UV-328
Portugal, Nov. 2010	raw wastewater	24	26	85	76
	treated wastewater	n.d.	n.d.	31	21
Spain, Jan. 2011	raw wastewater	n.d.	40 (6)	n.d.	53
	treated wastewater	n.d.	n.d.	n.d.	n.d.
Spain, Feb. 2011	raw wastewater	n.d.	34	22	65
	treated wastewater	n.d.	n.d.	n.d.	n.d.

n.d. = not detected

Carpinteiro et al. (Carpinteiro et al., 2012a) also measured benzotriazole UV-absorbers in sediments. Matrix solid-phase dispersion followed by gas chromatography tandem mass spectrometry was used. The limit of quantification of the method was 3 ng/g for UV-320, -326, -327 and -328. Ten samples of river and estuarine sediments with different carbon contents were investigated. Fresh sediment samples were air-dried in the hood for several days then sieved. The fraction with the particle size < 0.3 mm was considered in the study. In 6 of the 10 sediment samples quantifiable levels of UV-absorbers were detected:

Table 28: Concentrations of benzotriazole UV-absorber species measured in sediment samples (paricle fraction < 0.3 mm, n=3 replicates, - = not detected)

Sample	total carbon [%]	UV-320 [ng/g]	UV-326 [ng/g]	UV-327 [ng/g]	UV-328 [ng/g]
1	3.0	5.6	32	15	56
2	3.9	-	-	10.3	10
3	5.5	-	7.8	-	8.3
4	4.6	-	-	9.5	11.2
5	2.2	-	-	-	7.9
6	8.0	-	15	-	8

Unfortunately the origin of the sediment samples is not mentioned in the study. According to the acknowledgements some of the analyzed sediment samples were supplied by the German Federal Institute of Hydrology. However, the authors could not specify which samples were from Spain and which were from Germany (personal communication April 2012).

Montesdeoca-Esponda et al. (Montesdeoca-Esponda et al., 2012) used on-line solid-phase extraction coupled to ultra-performance liquid chromatography with tandem mass spectrometry detection (SPE-UPLC-MS/MS) for the determination of UV-326, -327, -328, -329, -360 and -571 in samples from WWTP effluents and coastal marine water from Spain. The detection limits and quantification limits achieved were in the range of 0.6-4.1 ng/L and 2.1-14 ng/L. The analytical method allowed simultaneous determination of the compounds in liquid samples with satisfactory recoveries and reproducibility, except for UV-360, which cannot be completely eluted from the cartridge due to its high octanol-water partition coefficient and molecular mass.

Seawater samples were collected from six beaches around the Gran Canaria Island in Spain (2 samples per beach), wastewater samples were collected from seven WWTPs of Gran Canaria Island. All substances studied were detected in the wastewater samples (see table). In seawater samples only UV-360 was found (6 of 12 samples, 3.6 – 5.2 ng/L).

Table 29: Concentrations of phenolic benzotriazole UV-absorbers in samples of WWTP effluents of Gran Canaria Island

	detection frequency	**concentration(s) [ng/L]**
UV-326	1/7	11
UV-327	1/7	4.8
UV-328	5/7	6.2 – 13
UV-329	1/7	4.0
UV-360	2/7	5.9 and 6.6
UV-571	0/7	not detected

Soil and suspended solids samples from the German Environmental Specimen Bank were analyzed for UV-234, -320, -326, -327, -328, -329 and -350 at the University of Santiago de Compostela (Rodríguez Pereiro and Casado Agrelo, 2012). Samples were extracted using the matrix solid-phase dispersion (MSDP) technique, with an integrated clean-up step. A GC-MS/MS method was used with a hybrid quadrupole time-of-flight mass spectrometer furnished with an electronic impact source. The limits of quantification were 2 ng/g per compound.

Samples were from sites with high anthropogenic influence and from background sites. Five soil samples taken in 2010 and five samples of suspended particulate matter taken in 2011 were analyzed. Soil samples were 3 litter samples, one root network sample and one top soil sample. All soil samples revealed target compound levels below the limits of quantification, also for the soils from Saarbruecken-Staden (root network) and Duebener Heide/Leipzig (litter, top soil) which are assumed to be more anthropogenically influenced. Concentrations of phenolic benzotriazoles in suspended solids samples are shown in Table 30.

Table 30: Concentrations of phenolic benzotriazoles in suspended solids samples from Germany

Suspended solids sample	**UV-234 [ng/g dw]**	**UV-320 [ng/g dw]**	**UV-326 [ng/g dw]**	**UV-327 [ng/g dw]**	**UV-328 [ng/g dw]**	**UV-329 [ng/g dw]**	**UV-350 [ng/g dw]**
Danube / Jochenstein	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Rhine /Weil	n.d.	n.d.	26	n.d.	26	n.d.	n.d.

Elbe / Cumlosen	8.1	n.d.	4.6	n.d.	n.d.	n.d.	n.d.
Saale / Wettin	15	n.d.	17	n.d.	n.d.	n.d.	n.d.
Saar / Rehlingen	17	n.d.	17	n.d.	n.d.	2.0	n.d.

n.d. = not detected

Suspendid solids from the river Elbe and its tributary Saale showed similar patterns, with higher levels for the tributary Saale. Patterns for suspended solids from the rivers Saale and Saar are comparable. Both rivers revealed high burdens also for other substances. The Rhine site Weil downstream Basel is influenced by the Swiss chemical industry and has a different pattern (higher level of UV 326, only site with UV 328). The Danube site at Jochenstein was selected because of low burdens and displayed levels below the limits of quantification.

Japanese studies:

Nakata et al (Nakata et al., 2009a) studied occurrence and concentrations of UV-320, -326, -327 and -328 in marine organisms and sediments from the Ariake Sea, western Japan. 16 coastal and river sediments were collected during 2006-2007. Five of the sediment samples were taken in a heavily polluted river. 55 biota samples were collected during 2004 and 2007:

- tidal flat organisms: lugworm, lamp shell, oyster, clam, gastropod, crustaceans (crab, shrimp), fishes (herbivorous and omnivorous mudskippers)
- shallow water species: crustaceans (crab, shrimp), teleost fish (flathead, solefish, right eye flounder, sandperch, sweetlips, mullet, sea bass, hairtail), cartilaginous fish (eagle ray, hammerhead shark)
- coastal birds (spot-billed duck, mallard).

Depending on the species, the whole body, soft tissue, hepatopancreas and liver samples were analyzed. 16 coastal and river sediments were also collected around the Ariake Sea during 2006-2007. UV-stabilizers were detected in all biota and sediment samples. In biota UV-326, -327 and -328 were the dominant compounds at levels of 0.1-55 ng/g ww. Concentrations of UV-320 in samples were low, it could be detected only in tidal flat organisms and some shallow water species. This may be due to small amounts of use of this compound in Japan since its domestic production and use have been restricted.

In general, concentrations of UV-stabilizers in tidal flat organisms were greater than those in shallow water species. The average concentrations of UV-320 and UV-326 in tidal flat species were approximately 10- to 20-fold higher than those in shallow water organisms. The tidal flat clam showed the highest concentrations of UV-320 and UV-326 at 74 ng/g and 219 ng/g (lw) respectively. Elevated concentrations of UV-326 were also found in oysters and gastropods in tidal flat area. These results imply the presence of phenolic benzotriazoles in sediment, resulting in accumulation of these compounds in benthic organisms. The low concentrations of UV-326 in shallow water species might be explained by low BCF of this compound, as compared with other benzotriazole UV-filters. In addition the authors speculate that biodegradation of UV-326 in shallow water organisms may be a possible reason for low accumulation of this compound.

UV-327 was most frequently detected in the organisms investigated. The average concentrations of UV-327 in tidal flat organisms were only 2-fold higher than those in shallow water species. The tidal flat clam, crab and herbivorous mudskipper contained high concentrations of UV-327 (> 100 ng/g lw), followed by gastropods and oysters. In shallow water fishes such as mullet, sea bass and young sea bass, concentrations of UV-327 were 3- to 4-fold higher in liver than in carcass. These results are consistent with the concentration profiles of UV-328 in mullet, suggesting the preferential accumulation and less biodegradation of this compound in the liver of some fish species. Omnivorous birds accumulate UV-327 in the liver, at average concentrations of 90 ng/g (lw) in a spot-billed duck and 59 ng/g in mallards. This suggests bioaccumulation in higher trophic species in the aquatic food chain.

Concentrations of UV-328 in biota were variable and species-specific. The highest concentration was found in tidal flat gastropod at 460 ng/g (lw), followed by mullet (120 ng/g lw in whole body and 250 ng/g lw in liver) and hammerhead shark (130 ng/g lw in liver) collected from shallow waters. The oysters and clams in tidal flat contained high concentrations of UV-328, at >100 ng/g lw. The large variations in UV-328 concentrations observed in this study might be due to differences in retention and metabolism of this compound in marine organisms.

As described above, the concentrations of benzotriazole UV-stabilizers in tidal flat organisms were higher than those in shallow water species. In addition, clams, oysters and gastropods presented high concentrations of UV-320, UV-326 and UV-328 rather than crabs and fishes, although the former species are at lower trophic levels in the tidal flat ecosystems. There is no positive correlation between the concentrations and the trophic status of organisms in marine ecosystems.

The benzotriazole UV-stabilizers were detected in 11 coastal sediments analyzed, at total concentrations of several ng/g dw. UV-328 was found at the highest concentrations (average 6.4± 4.0 ng/g dw), followed by UV-326 (3.7 ± 3.0 ng/g dw), UV-327 (3.2 ± 2.6 ng/g dw) and UV-320 (0.9 ± 0.6 ng/g dw). The composition of the UV-stabilizers among the sediment samples was less variable than in biota. Extremely high concentrations were found in five sediments from the highly polluted Omuta River. Highest concentrations of UV-320, -326, -327 and -328 reached 14, 200, 190 and 320 ng/g dw, respectively. Significant correlations were found in sediment concentrations between UV-326 and 327, UV-326 and 328, and UV-327 and 328 in the Ariake Sea. Significant correlations were also found between UV-stabilizer concentrations and organic carbon contents in sediment.

Table 31: Concentrations of benzotriazole UV-stabilizers in tidal flat and shallow water organisms collected in Japan

	UV-320 [ng/g ww]	**UV-326 [ng/g ww]**	**UV-327 [ng/g ww]**	**UV-328 [ng/g ww]**
10 tidal flat organisms	< 0.05 – 0.60	< 0.10 – 2.5	< 0.12 – 3.6	0.35 - 14
10 marine shallow water organisms	< 0.05 – 0.09	< 0.10 – 0.32	< 0.12 – 2.3	0.19 – 8.7
6 marine shallow water organisms (liver)	< 0.05 – 7.0	< 0.10 – 5.6	2.4 - 13	< 0.15 - 55
2 species of water fowl (liver)	< 0.05	< 0.10	2.6 3.4	< 0.15

Table 32: Concentrations of benzotriazole UV-stabilizers in sediments in Japan

	UV-320 [ng/g dw]	UV-326 [ng/g dw]	UV-327 [ng/g dw]	UV-328 [ng/g dw]
marine and estuarine sediments (n = 11)	0.3 – 2.3	1.5 - 12	1.6 – 9.9	7.9 - 40
Omuta River sediments (n = 5)	2.6 - 14	23 – 200	16 – 190	18 - 320

Nakata et al. (Nakata et al., 2009b) also investigated occurrence and concentrations of UV-320, 326, 327 and 328 in marine organisms collected from the Ariake Sea, western Japan. 51 marine organisms, such as lugworms, mussels, oysters, crustaceans, fish, birds and marine mammals were collected during 2001 and 2005. 12 sediments were collected from the same region in 2007. Analyses were done via GC-MS.

UV-filters were detected in most marine organisms in the study. Highest concentrations were found in lower benthic organisms, gastropods, collected from the tidal flat area (UV-328 > 400 ng/g lw). UV-328 and -326 were the dominant components in these organisms. In shallow water species, elevated levels were found in the liver of mullet, a benthic fish (UV-328 > 200 ng/g lw). Higher trophic species, such as sharks, marine mammals and birds accumulate organic UV-filters. UV-328 and -327 were dominant in finless porpoises and mallards, respectively. The results suggest significant bioaccumulation of UV-filters through the marine food-webs.

The substances were also detected in surface sediments from the Ariake Sea (average concentration: several ng/g dw). High concentrations of UV-filters were found in the Omuta River sediments, at levels ranging from 2.3-320 ng/g dw. Significant correlations were found between concentrations and organic carbon contents in sediments. No more details are given.

In order to understand the geographical distribution of UV-filters, blue and green mussels from 10 Asian countries and regions were collected during 1998 and 2005 and analyzed (Cambodia, China, Hong Kong, India, Indonesia, Japan, Korea, Malaysia, the Philippines, Vietnam). Only qualitative information is given on this investigation. UV-filters were detected in most mussel samples, indicating the widespread use of these compounds in Asian coastal regions. In general, UV-326 was the dominant compound, whereas UV-320 was detected only in several samples collected from Japan. The UV-filters concentrations were high in mussels from Korea, Japan and Hong Kong. Low residue levels of UV-filters were found in samples from India and Vietnam. These results suggest different usage values of UV-filters among countries and regions in Asia. Concentrations in mussels showed great spatial variations in Korea and Japan, which may be due to the distance between the sampling points and the sources of UV-filters, such as WWTPs. Significant positive correlation was determined in concentrations between UV-327 and UV-328 in mussels.

Nakata and Shinohara (Nakata and Shinohara, 2010) analyzed UV-320, -326, -327 and -328 in influent, effluent and sewage sludge samples collected from 5 WWTPs located in a town (population 680,000) in Japan. Samples were taken in May and October 2009. The wastewater flows were 140,000, 29,300, 9,300, 53,300 and 63,200 m^3/d, respectively. The treatment process included activated sludge method in all WWTPs. In the biggest WWTP (East WWTP) influent samples were collected at 9:00, 12:00, 15:00, 18:00 and 21:00 (n = 5), to study time-dependent variations of target substance concentrations. Influent and effluent samples were also obtained from the 4 other WWTPs (n = 1 / sample). Two sewage sludge samples were also collected from each of the five WWTPs (n = 10). The detection limits ranged from 2.1 to 8.7 ng/L in this study (limits of quantification not given).

Benzotriazole UV-stabilizers were detected in all influents collected from East WWTP at every three hours during 9:00 to 21:00. UV-326 showed the highest concentrations in influents, followed by UV-328 and -327.

Table 33: Concentrations [ng/L] of benzotriazole UV-stabilizers in influents of East WWTP

Time of sampling	9:00	12:00	15:00	18:00	21:00	Average ± standard deviation
UV-326	26	24	23	19	28	24 ± 3.7
UV-327	17	11	10	20	5.6	12 ± 5.6
UV-328	23	20	17	14	15	18 ± 3.9

Table 34: Concentrations of benzotriazole UV-stabilizers in five WWTPs in Japan

Concentration in	UV-326	UV-327	UV-328
influent (9 samples) [ng/L]	24 - 78	< 8.7 - 12	18 - 52
effluent (5 samples) [ng/L]	3.0 - 4.5	< 8.7	2.1 – 2.9
sludge (10 samples) [ng/g dw]	760 - 1800	120 - 200	430 - 570

Benzotriazole UV-stabilizers were detected in most samples analyzed and UV-326 was the dominant compound in influents (mean: 46 ng/L), followed by UV-328 (34 ng/L). UV-327 was detected in two influents at concentrations of 9.2 and 12 ng/L. UV-320 was not identified in any of the samples, probably because its domestic production and use have been restricted in Japan. These results imply a large amount of production and usage of UV-326 compared with other benzotriazole UV-stabilizers in Japan. Concentrations in the effluents were generally < 5 ng/L, suggesting an elimination of these compounds during wastewater treatment. The removal rates of UV-326 and -328 were >90% in the effluents, but high concentrations of benzotriazole UV-stabilizers were detected in sewage sludge samples of WWTPs, at high levels indicating adsorption to organic carbon in sewage sludge. The mean carbon percentage of sewage sludges was 31 ± 2.2 %. Partition coefficients (Kp) were calculated at a moisture content of 80% in sludges. The values are 7,200 ± 3,900 L/kg for UV-326 and 4,200 ± 970 L/kg for UV-328.

Nakata et al. (Nakata et al., 2010) also detected benzotriazole UV-stabilizers in the blubber of marine mammals. They analyzed UV-320, -327 and -328 in finless porpoises (*Neophocaena phocaenoides*) collected from the Yatsushiro Sea, Ariake Sea and Tachibana Bay, Japan, in 1999, 2008 and 2009, respectively. All animals were stranded or accidentally caught by fishing net. Detection limits were 0.05, 0.12, 0.15 ng/g for UV-320, -327 and -328, respectively.

Table 35: Concentrations of benzotriazole UV-stabilzers [ng/g ww] in the blubber of finless porpoises

sample no.	1	2	3	4	5
sampling year	1999	1999	2008	2009	2009

lipid content [%]	81	83	87	59	91
UV-327	4.5	9.5	6.3	31	18
UV-328	20	64	11	34	16

UV-320 was not detected in the samples, which is attributed to its restriction in Japan in 2007. The mean concentrations and standard deviations of UV-327 and UV-328 in five blubber samples were 19 ± 19 ng/g lw and 38 ± 28 ng/g, respectively, reflecting the higher consumption of UV-328 in Japan.

The authors cite a study showing a high concentration of UV-327 in the liver of a common cormorant (220 ng/g) collected from Hokkaido, northern Japan (respective reference in Japanese). While the concentrations of UV-327 in finless porpoises were lower than those in seabirds, the occurrence of UV-327 in marine mammals suggests the potential bioaccumulation in higher trophic species through the aquatic food chain.

According to the authors it has been reported that UV-327 concentrations in seawater from four coastal areas of Tokyo Bay were less than 0.5 ng/L and that the geometric mean concentration in river, lake and coastal water samples (n = 44) was 0.12 ng/L (respective references in Japanese). On the basis of these water concentrations the BAF of UV-327 between water and finless porpoises was estimated to be 33,300. Applying the same water concentrations to the calculation of a BAF of UV-327 in small fish inhabiting the same regions results in a value of 3250, which is comparable to the values found under laboratory conditions (3400 to 9000).

UV-328 was not detected in the liver of seabirds, although UV-327 was present in the samples (Nakata et al. 2009b). The log K_{ow} of UV-328 is the highest (8.28 reported in study) among the analyzed substances, but the BCF in fish was relatively low, 570-1400 and 620-2700 at the exposure concentrations of 0.1, 0.01 for 60 day, respectively (respective reference in Japanese). However, UV-328 showed a very high BCF, 36,000, between water and innards of fish (respective reference in Japanese). The authors conclude that the bioaccumulation profiles of UV-328 in marine organisms might be related to different retention and metabolism of this compound among species. The occurrence of UV-328 in finless porpoise may imply a low potential for biotransformation of this compound in this species. Finally it is stated that benzotriazole UV-stabilizers appear to be persistent and bioaccumulative in the aquatic food chain.

Kameda et al. (Kameda et al., 2011) measured 18 sun-blocking agents, among them UV-234, -326, -327, -328 and -329 in water and sediment collected from 22 rivers, 4 WWTP effluents and 3 lakes in August and September 2008 in Japan. Phenolic benzotriazoles are the most widely used UV-light stabilizers in Japan. WWTP sediment samples were collected from the river at the point of WWTP effluent discharge. In order to estimate contribution of sun-blocking agents from domestic wastewater to those in surface water and sediment, an indicator chemical for domestic wastewaters and WWTP effluents was also measured (HHCB = 1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethyl-cyclopenta-[g]-2-benzo-pyrane, a polycyclic musk, CAS 1222-05-5). The sampling sites represent 5 different groups:

- 2 streams with direct inputs of domestic wastewater (S1,S2)
- 4 WWTP effluents (ST1-ST4), conventional activated sludge treatment plants,
- 6 rivers heavily polluted by industrial and domestic wastewaters (H1-H6),
- 12 moderately contaminated rivers (M1-M12),

- 2 little rivers and 3 lakes as background sites (BG1-BG5).

Background sites did not receive domestic or industrial wastewater, but have possible slight sources (atmosphere deposition, recreational activities). In spite of considerable care, UV-328 was detected in blank samples. According to the authors this contamination was caused by analyte in indoor floor dust in the laboratory during experiments. The measured concentrations were corrected by the use of blanks upon each analysis. The limits of detection ranged from 0.1 ng/l to 3.0 ng/l and from 0.05 ng/g dw to 1.0 ng/g dw except for UV-328 which had a LOD of 10 ng/g dw.

The profiles of sun-blocking agents in surface water demonstrated site-specific differences at each sampling site. UV-328 was one of the dominant sun-blocking agents measured in water samples from heavily and moderately polluted rivers. The maximum level of UV-328 in heavily polluted rivers was near the lowest chronic NOEC of the substance estimated by EPI Suite (7 µg/L). UV-234 and UV-329 were neither detected in water samples from surface waters nor from WWTP effluents. At the background sites none of the phenolic benzotriazoles analyzed were found in water samples.

Table 36: Concentrations of phenolic benzotriazoles in water samples. UV-234 and 329 were not detected.

analyte		**UV-326**	**UV-327**	**UV-328**
streams (S1, S2)	Occurrence	1/2	1/2	1/2
	mean detected [a] [ng/L]	16	5	70
	range [ng/L]			
WWTP effluents (ST1-ST4)	Occurrence	1/4	1/4	3/4
	mean detected [ng/L]	13	2	62
	range [ng/L]			47-88
heavily polluted rivers (H1-H6)	Occurrence	1/6	1/6	4/6
	mean detected [ng/L]	9	1	701
	range [ng/L]			149-4780
moderately polluted rivers	Occurrence	5/12	6/12	8/12
(M1-M12)	mean detected [ng/L]	2	1	152
	range [ng/L]	1-22	1-6	30-583
background sites (BG1-BG5)	Occurrence	0/5	0/5	0/5
	mean detected [ng/L]			
	range [ng/L]			

[a] geometric mean calculated from detected samples

Table 37: Concentrations of phenolic benzotriazoles in sediment samples

analyte		**UV-234**	**UV-326**	**UV-327**	**UV-328**	**UV-329**
streams	Occurrence	1/2	2/2	2/2	2/2	1/2

(S1, S2)	mean detected [a] [µg/kg[b]]	1266	7.8	4.7	102	16
	range [µg/kg[b]]		0.1-110	0.6-37	10-1146	
WWTP effluents (ST1-ST4)	Occurrence	0/4	4/4	4/4	3/4	0/4
	mean detected [µg/kg]		0.8	0.5	13	
	range [µg/kg]		0.4-5.4	0.3-1.0	10-85	
heavily polluted rivers (H1-H6)	Occurrence	4/6	5/6	5/6	6/6	3/6
	mean detected [µg/kg]	99	4.7	2.4	117	26
	range [µg/kg]	38-324	0.9-45	0.7-18	21-1735	7.4-269
moderately polluted rivers (M1-M12)	Occurrence	8/12	12/12	10/12	9/12	3/12
	mean detected [µg/kg]	47	1.8	0.9	59	0.6
	range [µg/kg]	18-315	1.0-5.0	0.4-2.6	10-213	0.1-4.3
background sites (BG1-BG5)	Occurrence	3/5	2/5	2/5	3/5	0/5
	mean detected [µg/kg]	39	1.2	0.7	58	
	range [µg/kg]	8.3-113	1.1-1.3	0.5-1.1	29-89	

[a] geometric mean calculated from detected samples
[b] µg/kg dw

UV-234, -326, -327 and -328 were detected in most sediments. The compositions of sun-blocking agents in sediment were quite similar among the five sampling site groups. The highest geometric mean concentrations of 18 sun-blocking agents in sediments were detected in streams and in heavily polluted rivers. The highest contributions to the total concentrations were those of UV-234 and -328. These two substances accounted for 70-80% of the total contaminants identified at all sediment sampling sites.

The results demonstrate that high concentrations of phenolic benzotriazoles were accumulated in sediment receiving not only chemical plants effluent, but also residential wastewaters, WWTP effluent and surface runoff.

UV-234, -326, -327 and -328 were significantly correlated with HHCB in sediments from rivers and lakes. According to the authors this shows that a large input of these substances is from domestic wastewater or WWTPs. It also suggests that their behavior in rivers and lakes, such as partitioning and attenuation, is similar to that of HHCB. UV-329 had no significant correlation with HHCB in sediments.

UV-326 had a strong linear correlation between UV-327 as well as UV-328 in all sediments. Since UV-stabilizers are often used as mixtures, the ratios observed in sediments may reflect their compositions in the products. The authors suggest that their (degradation) behavior may be also quite similar.

In a presentation Nakata (Nakata, 2011) showed graphs with concentrations of UV-326, -327 and -328 in mussels from 10 Asian countries and in mussels from the USA mussel watch program. All data cited are taken from the graphs. 45 samples were taken during 2003 and 2005.

UV-326 was detected in mussels from 7 of the 10 Asian countries. Highest concentrations were detected in mussels from Japan and Korea (ca. 1.5 and ca. 1.2 µg/g lw, respectively). UV-327 was detected in 6 of the 10 countries with highest concentrations in Hong Kong and Korea (ca. 0.3 µg/g lw). UV-328 was detected in 8 of the 10 countries with highest concentrations in Hong Kong and Korea (ca. 0.8 µg/g lw).

In the USA samples were taken from blue mussels at 17 locations (n = 34) on the west coast (Alaska, Oregon, California) in 1994/95 and 2004/05. UV-326 and -327 were detected in most samples (14/17). Concentrations of UV-326 were similar to those measured in Japan and Korea. However, the maximum concentration was lower (ca. 0.7 µg/g lw). Concentrations of UV-327 were higher than in Japan, but slightly lower than in Korea and had a maximum of ca. 0.25 µg/g lw. UV-328 was detected in few samples, only, and showed a maximum of ca. 0.3 µg/g lw.

In an article Nakata et al. (Nakata et al., 2012) published more details on the mussel analyses. However, some more samples were included and other samples were excluded, so the results published in the article differ somewhat from those given in the presentation. Compounds analyzed were UV-320, -326, -327 and -328. 53 samples of blue and green mussels were collected from Cambodia, China, Hong Kong, India, Indonesia, Japan, Korea, Malaysia, Philippines and Vietnam during 2003 and 2007. In addition the analysis comprised 15 samples of blue mussels from the Pacific coast of the USA collected during 2004 and 2005. Liquid extraction and GC-MS in selective ion monitoring (SIM) mode was used. The limits of detection are given as 0.05, 0.1, 0.12 and 0.15 ng/g ww for UV-320, -326, -327 and -328, respectively.

Table 38: Mean concentrations of phenolic benzotriazoles in blue and green mussels [ng/g lw]. Geometric means in parenthesis.

	UV-320		**UV-326**		**UV-327**		**UV-328**	
Cambodia	0/2	n.d.	0/2	n.d.	0/2	n.d.	2/2	120 (110)
China	0/5	n.d.	2/5	60 (33)	4/5	84 (65)	3/5	96 (52)
Hong Kong	0/8	n.d.	2/8	91 (18)	6/8	93 (48)	6/8	200 (75)
India	0/3	n.d.	0/3	n.d.	0/3	n.d.	0/3	n.d.
Indonesia	0/2	n.d.	1/2	33 (22)	2/2	58 (45)	2/2	120 (110)
Japan	4/7	33 (13)	7/7	450 (260)	3/7	38 (15)	7/7	120 (93)
Korea	0/17	n.d.	13/17	210 (90)	11/17	100 (56)	16/17	220 (150)
Malaysia	0/4	n.d.	1/4	42 (12)	0/4	n.d.	1/4	24 (14)
Philippines	0/2	n.d.	1/2	120 (50)	2/2	150 (150)	2/2	170 (140)
USA	0/15	n.d.	12/15	130 (79)	11/15	61 (45)	3/15	69 (33)
Vietnam	0/3	n.d.	0/3	n.d.	0/3	n.d.	0/3	n.d.

Analytical results demonstrate ubiquitous contamination and widespread distribution of phenolic benzotriazoles. Levels were comparable to those of PCBs, DDTs and PBDEs. However, spatial variation of the concentrations was often high. Significant correlations were found between the concentrations of several phenolic benzotriazoles, which suggests similar sources and compositions of these compounds in commercial and industrial products. While Kameda et al. (2011) reported correlations of UV-326, -327 and -328 with the polycyclic musk HHCB, such correlations were not always found by Nakata et al. (2012). HHCB is an indicator substance for WWTP effluent. It is concluded that in addition to WWTP effluents there may be point sources or other sources, e.g. road dust, influencing the phenolic benzotriazoles concentrations in mussels.

The authors report that the domestic production and import of UV-327 in Japan decreased dramatically from 2436 tons between 2004 and 2009 to only 3 tons in 2010. They assume that this is due to the availability of an alternative in the Japanese market.

Yanagimoto et al. (Yanagimoto et al., 2011) studied the occurrence of UV-327 and -328 in human adipose tissues collected from Japan (2004-2005, n = 22), South Korea (2005-2006, n = 18), China (2002, n = 12), India (2008, n = 5), Spain (2006, n = 12), Poland (1990, n = 12) and the USA (2003-2004, n = 24). In addition foodstuffs collected from Japan were analyzed for UV-326, -327 and -328 (seafood, meat, eggs, vegetables, dairy products, potatoes, pulses, cereals, fruits, n = 32). Some of the foodstuffs originated from other countries than Japan. GC-HRMS/LRMS was used. All data cited are taken from graphs.

The highest concentrations in human adipose tissue were found In Japan and South Korea. In Japan up to ca. 60 ng/g lw UV-327 were detected in human adipose tissues, in South Korea the concentrations reached ca. 45 ng/g, whereas those in Europe were lower (up to ca. 17 ng/g in Spain, up to ca. 11 ng/g in Poland). Lowest concentrations were observed in the USA (up to ca. 5 ng/g lw). Concentrations of UV-328 were generally lower than those of UV-327: up to ca. 35 ng/g lw in Japan, up to ca. 20 ng/g in South Korea and up to ca. 6 ng/g in Spain, whereas UV-328 was not detected in samples from Poland and only in few samples at low concentrations in the USA (up to ca. 2 ng/g lw). No gender- and age-related differences in concentrations were observed.

In foodstuffs ubiquitous contamination with benzotriazole UV-stabilizers was found. Highest concentrations were detected in seafood (up to ca. 1.2 ng/g ww UV-326, 1.4 ng/g UV-327 and 1.7 ng/g UV-328) and meat (up to ca. 1.5 ng/g ww UV-326, 1.2 ng/g UV-327 and 1.0 ng/g UV-328). Meat with high concentrations was imported from the USA and Australia. Lower concentrations were detected in vegetables (up to ca. 1.0 ng/g ww UV-326, 0.3 ng/g UV-327 and 0.2 ng/g UV-328) and some fruit (up to ca. 0.5 ng/g ww each UV-326, 327 and 328). In dairy products no benzotriazole UV-stabilizers were found. The estimated daily intake of benzotriazole UV-stabilizers through food consumption was 861 ng/person/d. Contamination was mainly due to meat and vegetables (> 50%), which may imply the transfer of benzotriazole UV-stabilizers from plastic trays and wraps.

By way of a poster Nakata et al. (Nakata et al., 2011) reported temporal trends of UV-327 and -328 in archived marine mammal tissues. In addition temporal trends of UV-326, -327 and -328 in sediment cores were analyzed. Marine mammals sampled were finless porpoises and striped dolphins from Japanese coastal waters (n = 33). Sediment cores were taken from two sample stations at Tokyo Bay, Japan (n = 12). The sedimentation periods (1930-1999) were determined by ^{210}Pb and the particle fraction < 500 µm was investigated. All data cited are taken from graphs.

UV-327 and -328 were not detected in blubber samples collected around 1980, but in samples taken in 1990 and later. Maximum concentrations of UV-327 and -328 were ca. 45 ng/g lw and ca. 70 ng/g lw, respectively. An increasing trend is identified for UV-327 as well as UV-328.

Sediment cores showed an increasing temporal trend for UV-326, -327 and -328. Results are presented for two different sampling stations. At both sampling stations concentrations start to rise around 1970. Highest concentrations are found for UV-326 (maximum ca. 17 ng/g dw at station A, ca. 31 ng/g at station B), whereas concentrations of UV-327 and -328 were lower (UV-327 maximum ca. 8 ng/g dw at station A, ca. 4 ng/g at station B, UV-328 ca.10 ng/g at station A, ca. 4 ng/g at station B).

UV-320, -326, -327 and -328 were also detected in road dusts. Samples were collected in December 2010 at 9 stations of Route 57, Kumamoto, with a traffic density of approx. 5,000 to 60.000/d (Nakata Presentation, 2011). All data are taken from graphs.

Concentrations were low for UV-320 (n.d. - ca. 3 ng/g dw), higher for UV-328 (ca.2.5 - ca. 40 ng/g) and UV-326 (ca. 8 - ca. 55 ng/g) and at a single sampling point 116.9 ng/g UV-327 was detected (minimum ca. 8 ng/g dw). Concentrations of UV-320, -326 and -328 correlated with traffic density. The authors conclude that that automobile equipment might be a possible source of benzotriazole stabilizers in the environment.
Based on the data set obtained and the physicochemical properties of benzotriazole UV-stabilizers, the authors conclude that UV-327 will be a candidate of the POP Convention.

Watanabe and Noma (Watanabe and Noma, 2010) performed thermal treatment experiments using pilot-scale equipment and waste containing UV-320 as an input material to determine the destruction behavior of UV-320 and possible formation of UV-327 and NOx.

UV-320 was classified as a “Class I Specified Chemical Substance” under the Chemical Substance Control Law in Japan in 2007, which means that it is comparable in nature and toxicity to POPs (Watanabe and Noma, 2010). Manufacture and import of this substance have to be permitted, only specified uses are allowed and import of certain products specified by cabinet orders is prohibited. Therefore production, import and use of UV-320 have declined in Japan. However, it is still used in some countries, such as Korea and China and in Japan it may still be leached from long-life products. It is expected that incineration may be the predominant method of treatment for wastes containing UV-320.

Concentrations of UV-320 and -327 in “refuse derived fuels” obtained from Japanese municipal solid waste after removing the incombustible materials were 7.1 and 20 µg/kg, respectively. After treatment in the pilot-scale incinerator with two combustion units, bag filter, activated carbon adsorption tower and wet scrubber concentrations in the flue gas (final exit) were 0.0020 µg/m³ and 0.0042 µg/m³ for UV-320 and -327, respectively. Bottom ash contained 0.52 µg/kg UV-320 and 0.063 µg/kg UV-327, fly ash 0.36 µg/kg UV-320 and 0.049 µg/kg UV-327. After increasing the input concentration to 5000 mg/kg UV-320 concentrations of UV-320 and 327 in flue gas, bottom ash and fly ash were of the same order of magnitude as those observed at low input concentrations of UV-320.

UV-320 was destroyed mainly in the primary combustion zone. Overall destruction efficiency of UV-320 in input at a concentration of 5000 mg/kg was > 99.9999%. The input amount of UV-320 did not affect the formation and destruction behavior of UV-327 and NOx.

Other Asian studies:

Kim et al. (Kim et al., 2011b) developed a multiresidue analytical method for the determination of emerging pollutants including UV-234, -320, -326, -327, -328 and -329 in fish. The concentrations in fish muscle tissue were given on a lipid weight (lw) basis and the method detection limits were

0.3 – 9 pg/g for the UV-stabilizers mentioned above. Five individual fish samples belonging to three species of fish from Manila Bay, the Philippines were analyzed. Samples were collected during June 2008. Concentrations ranged from < method detection limit to 179 ng/g lw, suggesting the ubiquitous contamination in Manila Bay.

Table 39: Concentrations of phenolic benzotriazoles in fish muscle tissue [ng/g lw]

	bluetail mullet *V. buchanani* (n=1)	**coral grouper *E. corallicola* (n=1)**	**flathead grey mullet *M. cephalus* (n=3)**	
			mean	Min-Max
UV-234	not detected	14.3	34.6	22-47.1
UV-320	9.60	0.78	6.88	4.11-9.15
UV-326	211	n.d.	18.9	no data given
UV-327	2.57	18.5	14.6	10.5-18.5
UV-328	18.4	21.1	105	30.2-179
UV-329	not detected	39.4	7.29	6.69-7.89

Using the same method Kim et al. (Kim et al., 2011c) studied contamination of fish from Manila Bay, the Philippines, with benzotriazole UV-stabilizers including UV-234, -320, -326, -327, -328 and -329. Manila Bay is one of the pollution hot spots in the seas of East Asia with a very dense population and significant fisheries and aquaculture activities. It serves as a sink and transit area for the domestic and industrial wastes from metro Manila and the surrounding provinces. Many people depend on fish from the bay for food. During January and June 2008 58 fish specimens belonging to 20 species were collected from the local fish markets. Only fishes from Manila Bay were selected and analyzed. The method quantification limits were 1-27 pg/g lw.

Benzotriazole UV-stabilizers were detected, each at ng/g level in almost all fish samples, indicating ubiquitous contamination in coastal waters. Among the 8 targeted substances UV-328 was predominantly found with a mean concentration of 34.2 ng/g lw, implying large scale production and use of this compound in the Philippines. UV-328 was found in 88% of analyzed specimens (n = 58), UV-320 and UV-234 in 79% and 55%, respectively. UV-326, -327 and -329 were detected in less than half of the samples suggesting smaller amount of use or lower bioavailability. Generally concentrations of UV-320, -326, -327 and -328 in fish samples from the Philippines were higher than those reported in marine fish from shallow waters of Japan (Nakata et al., 2009a), which is attributed to large scale usage of the substances and/or the release of untreated wastewater containing the substances. In line with the results of Nakata et al. (2009a) concentrations of UV-320, though frequently detected, were lower than that of UV-234 and -328. According to the authors this may indicate the differences in accumulation and biodegradability of UV-320. Significant positive correlations were found between UV-234 and -328, UV-234 and -329, UV-320 and -327 and UV-320 and UV-328. From this it is suggested that fish in Manila Bay are exposed to benzotriazole UV-stabilizers originating from the same sources which are distributed homogenously in the bay. Examination of the relative contributions of each analyte to the total concentrations of analytes revealed that from the substances relevant for the SVHC dossier UV-328 was predominant. Compositions of the benzotriazole UV-stabilizers were different even in fishes belonging to the same family whereas some composition pattern was observed in fishes belonging to different families. This may be due to different availability, different metabolic capacity or selective uptake of the substances.

Concentrations of UV-234, -320, -326, -327, -328 and -329 did not show any relation with fish length and weight. Therefore, differences in accumulation/exposure pattern indicate the species specificity in fish samples. Concentrations measured in the different fish species varied greatly depending on the species within one to two orders of magnitude. This wide variation in concentrations indicates species-specific accumulation and elimination of the substances.

High concentrations of the sum of the investigated 8 substances were found in bumpnose trevally (*Caranoides hedlandensis*, n = 3), bluetail mullet (adult) (*Valamugil buchanani*, n = 1), common ponyfish (*Leiognathus equulus*, n = 3) and coral grouper (adult) (*Ephinephelus corallicola*, n = 1). These high concentrations (several hundred ng/g lw) indicate that these compounds are preferably accumulated by these species and/or that these species may have low metabolic capacity to eliminate benzotriazole UV-stabilizers. All these fishes belong to the demersal habitat.

Table 40: Concentrations of benzotriazole UV-stabilizers in marine species from Manila Bay, the Philippines

	lipid content [%]	UV-234 [ng/g lw]	UV-320 [ng/g lw]	UV-326 [ng/g lw]	UV-327 [ng/g lw]	UV-328 [ng/g lw]	UV-329 [ng/g lw]	Σ 8 benzotriazole UV-stabilizers
detection frequency [%]	---	55	79	19	43	88	41	---
Min. – Max. in 20 fish species (n = 58)	0.13-2.61	n.d. - 126	n.d. – 28.7	n.d. - 211	n.d. - 221	n.d. - 563	n.d. - 96.7	6.5 ± 11.1 - 316 ± 460

Kim et al. (Kim et al., 2012) used the same method for determining UV-234, -320, -326, -327 and -328 in house dust from the Philippines. During August 2008 house dust samples were collected from a residential area (Malate, n = 17) and near a large-scale open dumping area of municipal wastes (Payatas, n = 20) in Manila. People live directly at and even on the dumping area (http://www.dr-koelsch.de/html/payatas.html). House dust was collected in separate vacuum-cleaner bags used in each of the sampled house, which consist of dust from living room, kitchen and bedrooms. Dust was not collected from under furniture or in crevices between cushions. Obtained dust samples were combined individually for each house and sieved with a 500 µm mesh. Data on the details of the house, the possible sources of dust, floor area, number of computers/televisions, furniture and type of flooring were documented in a questionnaire at the time of sample collection.

Table 41: Concentrations of benzotriazole UV-stabilizers in house dust samples from Malate and Payatas in the Philippines

Target compounds	Malate					Payatas				
	DF[a] [%]	Median [ng/g]	Average [ng/g]	Min. [ng/g]	Max. [ng/g]	DF[a] [%]	Median [ng/g]	Average [ng/g]	Min. [ng/g]	Max. [ng/g]
UV-234	94	84	148	n.d.[b]	817	95	41	63	n.d.	212
UV-320	82	4.7	6.6	n.d.	25	65	3.0	6.9	n.d.	75
UV-326	88	50	53	n.d.	275	65	6.2	17	n.d.	133
UV-327	88	19	28	n.d.	73	80	10	10	n.d.	32

UV-328	82	27	50	n.d.	304	85	12	18	n.d.	48
Σ	---	147	285	n.d.	1020	---	118	115	n.d.	277

[a] DF: detection fequency
[b] n.d. = not detected

UV-234, -320, -326, -327 and -328 were frequently detected indicating ubiquitous contamination of the indoor environments. Among the target compounds, UV-234, -326 and -328 were the predominant compounds. The most abundant was UV-234, with a median value of 84 ng/g in Malate and 41 ng/g in Payatas. Significantly higher concentrations of UV-326 and -327 were found in house dust samples from Malate than those from Payatas, indicating possible differences in usage patterns of household products such as TV, waxes, coating materials, paints etc. between the two locations. Household products are considered the major source of contamination in the indoor microenvironment. The composition of phenolic benzotriazoles differed among the houses even within the same sampling region. It was not possible to distinguish the sources of the contamination. However, the correlations found for most of the benzotriazole UV-stabiliszers in house dust samples indicate a common source. This is in line with the results from other investigations (Kim et al.2011a, Nakata et al. 2009a)

Generally, levels of benzotriazole UV-stabilizers in dust from the Philippines are comparable to or lower than those measured by Carpinteiro et al. (2010b) in dust from Spain or the USA. Lower levels are attributed to lesser usage of the respective compounds in the Philipines.

Zhang et al. (Zhang et al., 2011) investigated UV-326, UV-327 and UV-328 in surface sediment samples (0-20 cm) collected from rivers in China (6 samples from river Songhua in 2009) and the U.S. (3 samples both from river Saginaw in 2002 and river Detroit in 1998). Five sewage sludge samples were collected from five WWTPs serving large cities located along the Songhua River in China in July 2009. Sediment and sludge samples taken from 4-6 spots within 10 m at a given sampling location were pooled to obtain a representative sample. UV-326, UV-327 and UV-328 were determined by use of a GC-MS.

The limit of detection (LOD) and the limit of quantification (LOQ) for sediment analysed in this study were 0.02 and 0.06 ng/g for UV-327 and 0.1 and 0.33 ng/g for both UV-326 and UV-328.The method LOD and LOQ values for sludge samples were 0.1 and 0.3 ng/g for UV-327 and 0.5 and 1.65 ng/g for both UV-326 and UV-328.

UV-326 was detected in 2 of 6 sediment samples from the Chinese River (1.71 and 2.01 ng/g dw) in 1 of 6 sediment samples from the U.S. (5.88 ng/g dw) and in all 5 sewage sludge samples from China (23.3-136 ng/g dw, mean 77.4 ng/g dw).

UV-327 was detected in 1 of 6 sediment samples from the Chinese River (0.310 ng/g dw) in 3 of 6 sediment samples from the U.S. (0.22-1.90 ng/g dw, mean 0.850 ng/g dw) and in 4 of 5 sewage sludge samples from China (1.80-8.40 ng/g dw, mean 3.68 ng/g dw).

UV-328 was detected in all 6 sediment samples from the Chinese River (2.06 - 7.12 ng/g dw, mean 3.81 ng/g dw) in 5 of 6 sediment samples from the U.S. (0.72-224 ng/g dw, mean 116 ng/g dw) and in all 5 sewage sludge samples from China (40.6-5920 ng/g dw, mean 1300 ng/g dw).

The concentration of UV-328 in sludge was the highest (mean: 1300 ng/g dw) among the target compounds.

Ruan et al. (Ruan et al., 2012) analyzed UV-234, -320, -326, -327, -328, -329 and -350 in municipal sewage sludge in China using an HPLC-MS/MS method. The method quantification limits were from 0.15 (UV-234) to 0.77 (UV-320) ng/g dw. Sixty sewage sludge samples from WWTPs in 33 cities were collected in 2010 and 2011. Most of the WWTPs are located in economically developed provinces in China. Samples were taken from freshly digested sludge at the dewatering process. The most dominant analogue was UV-234 at a median concentration of 116 ng/g dw. The abundance was successively followed by UV-329, -326 and -328 with median concentrations of 66.8, 67.8 and 57.3 ng/g dw respectively. UV-327 and UV-350 had low detection frequency, while UV-320 was not detectable in any sample. According to the authors the observed composition pattern in the sludge samples was quite consistent with the global production volumes of benzotriazole UV-stabilizers (according to the OECD and US EPA HPV databases).

Significant correlations were found among the phenolic benzotriazole concentrations and the daily treatment volume of the WWTPs was moderately correlated UV-329 and UV-328. Results from degradation prediction and multimedia fate simulation based on a quantitative structure-property-relationship (QSPR) model at screening level based on EPISuite and therefore comparable with the simulations done for the presented dossiers implied that the commercial benzotriazole stabilizers and their plausible transformation products might be persistent in the environment.

Table 42: Concentrations of benzotriazole UV-stabilizers in sludge from Chinese municipal WWTPs

Analyte	**Detection frequency**	**Concentrations [ng/g dw]**	**Median [ng/g dw]**
UV-234	58/60	0.96 – 235	116
UV-320	0/60	n.d.	-
UV-326	59/60	4.00 – 319 two extreme values: 2930 and 3390	67.8
UV-327	24/60	1.53 – 133	14
UV-328	58/60	3.54 – 213 one extreme value: 24,700	20.6
UV-329	59/60	0.57 – 757	66.8
UV-350	5/60	1.88 – 42.7	13.8

Australian studies:

Liu et al. (Liu et al., 2011b; Liu et al., 2012) developed a method for simultaneous determination of benzotriazoles and UV-filters (including UV-326 and -329) in ground water and WWTP effluent and biosolid samples using GC-MS/MS. The method was applied to screen the selected substances in samples from Bolivar WWTP in Adelaide, South Australia. The WWTP serves a population of 1,300,000 and is designed to have dry weather flow of 148.5 ML/d. About 75% of the inflow is from domestic sources, 25 % from industrial sources. The WWTP consists of primary sedimentation, secondary activated sludge treatment, stabilization lagoons and dissolved air flotation/filtration. The effluent is piped to a vegetable growing region for irrigation, or recharged into aquifer on site. The sludge line comprises mesophilic anaerobic digestion and sludge stabilization lagoons.

Groundwater samples were collected from an aquifer storage and recovery well at a depth of 300 m below ground within the WWTP site. Biosolid samples were collected from different sludge treated process (sludge is dewatered and dried using a combination of sludge drying lagoons, centrifugation and agitated air drying). 3 parallel samples were collected for each sample type.

In groundwater and effluent water concentrations of UV-326 and -329 were below the limits of quantification (LOQ). The LOQ were: 4.9 ng/L in tap water and 11.0 ng/L in effluent for UV-326 and 18.6 ng/L in tap water and 16.0 ng/L in effluent for UV-329. The concentration in biosolid samples was 49.9±7.4 ng/g for UV-326 (LOQ 1.1 ng/g) and 122.9±7.1 ng/g for UV-329 (LOQ 27.4 ng/g).

Results published in 2012 focus on the removal processes in the WWTP. 24 h composite water samples and samples of sludge (24 h composite or grab) and influent suspended solids were collected in April and October 2010. The average removal efficiencies of suspended solids, BOD_5 and NH_4-N were above 99% during the sampling periods. The highest value of LOD for the target analytes (4 benzotriazoles and 6 UV-filters including UV-326 and -329), were 16.3 ng/L in the influent, 14.1 ng/L in the effluent and 8.2 ng/g in biosolid samples.

All water and sludge concentrations are taken from graphs. UV-326 was detected in the influent in concentrations of ca. 35 ng/L (April) and ca. 20 ng/L (October), UV-329 in concentrations of ca. 230 ng/L (April) and ca. 420 ng/L (October). According to the authors both substances were completely removed from the water phase. However, removal rates of both > 100% and < 0% were noticed in some treatment stages, which might be due to variations in the input and output concentrations. Concentrations of UV-326 and UV-329 in influent suspended solids were always near 100 ng/g. Both substances are further detected in all other sludge samples taken after different treatment steps.

A mass balance analysis was applied to establish mass flux in the plant and removal mechanisms. However, few data were available, concentrations in water and sludge varied considerably with different treatment stages. The authors discuss plenty uncertainties associated with the mass balance analysis, but nevertheless state that sorption onto sludge played a dominant role in the removal of UV-326 in the WWTP whereas biological degradation played a significant role for UV-329.

American studies investigating the environmental impact of a certain industrial point source:

Jungclaus et al. (Jungclaus et al., 1978) analyzed industrial WWTP effluent and receiving waters and sediments from an American specialty chemicals manufacturing plant producing organic compounds and running a badly performing WWTP. 16 water samples and 19 sediment samples were taken in 1975 and 1976 and the compounds contained were identified, beside others UV-320, -327 and -328. River water and sediments were collected in Providence River and its tributary Pawtuxet River (Pruell et al., 1984).

UV-328 was detected in industrial WWTP effluent (0.55 – 4.7 ppm), in river water (7 – 85 ppb) and in sediments (1-100 ppm). UV-320 and UV-327 were detected only in sediment, with concentrations of 40 ppm and 2 – 300 ppm, respectively.

Lopez-Avila and Hites (Lopez-Avila and Hites, 1980) investigated transport of pollutants in sediments in the USA. The wastewater from a small specialty chemicals manufacturing plant located on the Pawtuxet River (Rhode Island) contaminated the water and sediment of that river, which flows into the brackish Providence River and Narragansett Bay. UV-328 had been manufactured in the plant since 1970. Wastewater samples from the clarifier tank, water samples and sediment cores were taken. Reported concentrations represent minimum values since they had not been corrected for solvent extraction efficiencies. Average water concentrations for UV-328 (geometric averages of 2-5 values measured at the specified locations at different times) were 3000 ppb in the wastewater of the plant, 40 ppb in river water near the plant, 10 ppb in more distant river water, 8-9 ppb in the mouth of the Pawtuxet River and 0.5-2 ppb in the Providence River. The concentrations follow the rules of simple dilution. UV-327 was manufactured at the plant between 1963 and 1972. It was not detected in any of the water samples.

Eight sediment cores were taken at three locations in the Pawtuxet River. The sites were selected for an abundance of fine-grained material. Further sediment cores were taken at 4 locations in the Pawtuxet Cove and 13 locations in the Providence River and Narragansett Bay. The core concentrations of the compounds in the sediment have been condensed into a single number. However, the authors feel the values given are representative of the sediment concentrations. Concentrations decrease both with depth in the sediment and with increasing distance from the discharge.

Table 43: Concentrations of phenolic benzotriazoles in sediment cores (ppm)

	Pawtuxet River			**Pawtuxet Cove**	**Providence River**		
	near plant	**mid river**	**near dam**		**near**	**far**	**bay**
UV-327	300	400	20	80	20	2	0.5
UV-328	300	300	70	100	10	5	0.6

Pruell et al. (Pruell et al., 1984) developed an analytical method for the determination of PAHs and phenolic benzotriazoles in clams. Concentrations of UV-327 and -328 were measured in hard shell clams (*Mercenaria mercenaria*) purchased from Rhode Island seafood stores in 1979. Personnel in nine of the 13 stores surveyed indicated that the clams were harvested from Narragansett Bay. Three seafood stores were sampled a second time to determine if the higher values obtained at these establishments were representative of their usual stock. As controls, clams were collected from a relatively unpolluted site in lower Narragansett Bay. The detection limit for specific compounds was ca. 0.1 ng/g ww.

The levels in purchased clams were generally higher than the concentrations found in clams collected from a lower Narragansett Bay control location. However, also in control samples both substances were detected. In summary UV-328 and UV-327 were present in clam tissue in concentrations ranging from 7 – 65 ng/g ww and from 1.0 – 8.5 ng/g ww (including controls). The ratio of UV-328 to UV-327 in clams varied from 2.7 to 9.5. This is similar to the ratio in surface sediments of the bay which ranges from 2.0 to 7.6. A significant correlation existed between UV-327 and UV-328.

Reddy et al. (Reddy et al., 2000) examined the free and bound fractions of different substituted benzotriazoles in sediment cores from the Pawtuxet River and Narragansett Bay in the U.S. The chosen benzotriazoles were produced from 1961 to 1985 by a major chemical plant located on the Pawtuxet River. Beside others, UV-326, -327 and -328 were investigated. Previous research has used these compounds as specific tracers of inputs from the Pawtuxet River into Narragansett Bay sediments and they are highly enriched in the sediments of both.

The Pawtuxet River sediment core was collected in 1989 and sectioned at 2-3 cm intervals. Eleven sections from 0-2 cm to 50-52 cm were analyzed. The sedimentation rates in this section of the river are 2-3 cm/year. The redox discontinuity, determined visually, was in the top 2 cm of the core. The Narragansett Bay core was collected in 1997. Six sections from the top 13 cm of the core were analyzed. The sediments in this area become anoxic within a few millimeters of the surface and have a sedimentation rate of about 0.3 cm/year. The deepest sections of both cores were the approximate depths of where the phenolic benzotriazoles were no longer detected and should roughly be equivalent to the initial date of production of these compounds (1961-1979). The method detection limit was ca. 20 ng/g for each (free and bound) fraction.

In the Narragansett Bay core UV-327 and -328 were detected at trace levels in the 10-13 cm section and their concentrations generally increased up-core (with concentrations as high as 25 µg/g). UV-326 was detected at much lower concentrations. UV-327 and -328 were not detected in the bound fraction in the Narragansett Bay core.

In the Pawtuxet River core all benzotriazoles were detected in the free fraction. UV-327 was most abundant: the highest concentration was ca. 5 mg/g and it was observed down to 50-52 cm. The other benzotriazoles were only present in the top 20 cm of the core. UV-326 and -327 were also found in the bound fraction of the Pawtuxet River core in at least the top 15 cm. However, the maximum percentage bound was 0.04%.

Benzotriazoles that had alkyl substitution in ortho position to the hydroxyl group were less likely to be found in the operationally defined bound fraction than compounds that did not have this substitution.

Hartmann et al. (2005) took sediment cores at three locations in Narragansett Bay in 1997 (Apponaug Cove, Seekonk River, Quonset Point). The cores were analyzed for several contaminants including UV-327 and UV-328. The phenolic benzotriazoles were used as markers indicating the years of their introduction (1963 for UV-327 and 1970 for UV-328). Two of the cores were split into 2 cm sections, and the third core (Quonset Point) was split into 10 cm sections.

Sharp breaks in the concentrations of UV-327 and UV-328 marking their introduction were successfully used to determine the sedimentation rate at Quonset Point. Both the Quonset Point and Seekonk River cores had subsurface maximums for phenolic benzotriazoles, which were consistent with expected inputs to the environment. The Apponaug Cove core showed an increase of the contaminants at the surface indicating a recent event in which more contaminated sediments were deposited at that location. The distributions of phenolic benzotriazoles at Apponaug Cove and in the Seekonk River indicate that there was a disturbance in the depositional environment relative to cores collected at these locations in 1986, demonstrating the potential for buried contaminants to be remobilized in the environment even after a period of burial.

At Quonset Point the phenolic benzotriazole profile increased down core through the 40-50 cm section before decreasing in the 50-60 cm section. Below the 50-60 cm section, UV-327 and UV-328 were below the detection limit of 10 ng/g dw. In the 50-60 cm section UV-327 is much more prominent than UV-328. Moving up core, UV-328 progressively accounts for more of the sum of both phenolic benzotriazoles. This reflects the earlier introduction (1963) and subsequent earlier discontinuation (1972) of UV-327 relative to UV-328 (1970 and 1985, respectively).

At Apponaug Cove surface concentrations were higher than the lower sections of the core. There could be degradation in the oxic surface layer of the sediments with subsequently lower concentrations in the deeper sections. However, data from a core taken in 1986 had a profile more consistent with the appearance of the different analytes. Therefore the authors assume that the distribution of phenolic benzotriazoles represents resuspended sediment transport and deposition of materials with high concentrations.

Data from the Seekonk River core also show high concentrations in the surface layer. Another core taken in the same area in 1986 showed a more orderly decrease down to 70 – 80 cm. The authors assume that some sedimentary layers were removed. Additional evidence of a disturbance is found in the ratio of the phenolic benzotriazoles. The lowest core section with phenolic benzotriazoles (12 – 14 cm) should have high ration of UV-327 to UV-328 due to their production history, but in this case actually had a lower ratio of UV-327 to UV 328 than the sections above it.

Table 44: Concentrations of phenolic benzotriazoles in sediment cores from Narragansett Bay (concentrations taken from a graph)

Quonset Point core			Apponaug Cove core			Seekonk River core	
depth [cm]	**UV-327 [ng/g dw]**	**UV-328 [ng/g dw]**	**depth [cm]**	**UV-327 [ng/g dw]**	**UV-328 [ng/g dw]**	**UV-327 [ng/g dw]**	**UV-328 [ng/g dw]**
0 - 2	ca. 40	ca. 160	0 - 2	ca. 130	ca. 270	ca. 30	ca. 120
0 - 10	ca. 60	ca. 260	2 - 4	ca. 30	ca. 80	ca. 20	ca. 70
10 - 20	ca. 80	ca. 360	6 - 8	ca. 50	ca. 140	ca. 30	ca. 140
20 - 30	ca. 100	ca. 840	10 – 12	ca. 70	ca. 120	-	-
30 - 40	ca. 130	ca. 1100	12 - 14	-	-	ca. 5	ca. 20
40 – 50	ca. 690	ca. 1180	20 – 22	n.d.	n.s.	n.d.	n.d.
50 - 60	ca. 480	ca. 40	30 – 32	n.d.	n.d.	-	-
60 - 70	n.d.	n.d.	38 – 40	-	-	n.d.	n.d.
80 - 90	n.d.	n.d.	40 – 42	n.d.	n.d.	-	-
100 - 110	n.d.	n.d.	48 - 50	-	-	n.d.	n.d.
119 - 129	n.d.	n.d.					

n.d. = not detected
- = not measured

At Apponaug Cove the phenolic benzotriazole profile indicates a much higher surface concentration than the lower sections of the core. Because the production of UV-328 was discontinued 12 years before the core was taken and the production of UV-327 25 years before that date, the authors attribute the high surface concentrations to resuspended sediment transport and deposition of materials in Apponaug Cove with relatively high concentrations of phenolic benzotriazoles. The ratio of UV-327 to UV-328 also increases in the surface section and may indicate a disturbance of older sediments having higher UV-327 levels.

ANNEX 6: AVAILABLE INFORMATION ON ENDOCRINE DISRUPTING PROPERTIES OF PHENOLIC BENZOTRIAZOLES

In-vitro-Studies

The estrogenic activity of several phenolic benzotriazoles was tested in a Yeast-Estrogen-Screen-assay (YES-assay) with human estrogenic receptors. In the study of Miller et al. (Miller et al., 2001) UV-327 and UV-329 (CAS 3147-75-9) were tested and in the study of Kawamura et al. (Kawamura et al., 2003) UV-327, UV-234 (CAS 70321-86-7), UV-326 (CAS 3896-11-5), UV-328 and UV-P (CAS 2440-22-4). Both studies showed that none of the phenolic benzotriazoles tested was triggering an estrogenic receptor activity.

In a study of Kunz et al. (Kunz et al., 2006) UV-360 (CAS 103597-45-1) was tested in a Yeast-Estrogen/Androgen-Screening-assay (YES/YAS-assay). No effects were reported.

In-vivo-Studies

In a recent review of the U.S. National Toxicology Program on the phenolic benzotriazoles UV-P, UV-329, UV-326, UV-320, UV-327, UV-328, UV-234, UV-360 as well as CAS 84268-36-0 (i.e. M1), 84268-33-7 (i.e. the methyl ester of M1), 84268-08-6 (i.e. a more complex ester of M1) and CAS 104810-48-2/104810-47-1 (i.e. an oligomeric ester of M1) (National Institute of Environmental Health Sciences, 2011) an overview over the available toxicity studies on mammals is given. There are several indications on effects mentioned that might be caused by endocrine disruption, e.g. reduced concentrations of testosterone, higher concentrations of CYP450, or higher activity of ethoxyresorufin-O-deethylase (EROD-activity). As in these cases there are also indications for toxic effects on the liver reported, the effects might actually be only secondary effects. With the present knowledge it is not possible to attribute them unambiguously as endocrine adverse effects.

Preliminary assessment of ED-properties for the phenolic benzotriazoles

There are several indications on effects of phenolic benzotriazoles mentioned that might be caused by endocrine disruption, e.g. reduced concentrations of testosterone, higher concentrations of CYP450, or higher activity of ethoxyresorufin-O-deethylase (EROD-activity). As in these cases there are also indications for toxic effects on the liver reported, the effects might actually be only secondary effects. With the present knowledge it is not possible to attribute them unambiguously as endocrine adverse effects of an equivalent level of concern.

ANNEX 7: ABBREVIATIONS

°C	Degrees centigrade
Å	Angstrom
avg.	Average
B	Bioaccumulative
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BOD_x	Biological oxygen demand in x days
BMF	Biomagnification factor
CAS	Chemical Abstracts Service
CLP	Classification, labelling and packaging (of substances and mixtures)
C&L	Classification and labelling
cm	Centimetres
cm^2	Centimetres squared
cm^3	Cubed centimetres
CMR	Carcinogenic, mutagenic, toxic to reproduction
CYP450	Cytrochrome P 450
d	Day
DDT	Dichlorodiphenyltrichloroethane
DegT50	Time interval after which 50% of a substance is degraded
DF	Detection frequency
DT_{50}	Time interval after which 50% of a substance is degraded or disappeared otherwise from the test medium
DisT50	Time interval after which 50% of a substance disappeared from the test medium (no degradation)
dw	Dry weight
EC	European Community
ECHA	European Chemicals Agency
EPA	Environmental Protection Agency
EROD	Ethoxyresorufin-O-deethylase
EU	European Union
g	grammes
GC	Gas chromatography
GC/MS	Gas chromatography – mass spectrometry
GC-MS/MS	Gas chromatography – tandem mass spectrometry
GC-HRMS/LRMS	Gas chromatography – high resolution mass spectrometry/low resolution mass spectrometry
GLP	Good laboratory practice
h	Hour
H 351	Classification: suspected of causing cancer
H 373	Classification: May cause damage to organs through prolonged or repeated exposure
H 412	Classification: Harmful to aquatic life with long lasting effects
HALS	Hindered Amine Light Stabilizers
HHCB	1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethyl-cyclopenta-[g]-2-benzo-pyrane, a polycyclic musk, CAS 1222-05-5
HPLC	High performance liquid chromatography

HPLC-MS/MS	High performance liquid chromatography – tandem mass spectrometry
IUPAC	International Union of Pure and Applied Chemistry
k	Rate constant (e.g. for biodegradation in sewage treatment plants)
$K_{air-water}$	Air-water partition coefficient
Kg	Kilograms
Km	Kilometres
Koc	Organic carbon-water partition coefficient
Kow	Octanol/water partition coefficient (log value)
Kp	Partition coefficient
KPa	Kilopascals
L (or l)	Litres
LC	Liquid chromatography
LC-MS	Liquid chromatography – mass spectrometry
LC-MS/MS	Liquid chromatography – tandem mass spectrometry
LC50	Lethal concentration for 50% of the test organisms
LOD	Limit of detection
LOQ	Limit of quantification
lw	Lipid weight
M	Molar
m^2	Metres squared (area)
m^3	Cubed metres (volume)
Max	Maximum
Min	Minimum
MITI	Ministry of International Trade and Industry (Japan)
mg	Milligrams
ml	Millilitres
ML	Megalitre
Mol	Moles
Mmol	Millimoles
MS	Mass spectrometry
µg	Micrograms
n	Number (e.g. number of samples)
n.d.	Not detected
NER	Non-extractable residues
NITE	National Institute of Technology and Evaluation, Japan
nm	Nanometres
NOEC	No-observed effect concentration
oc	Organic carbon
OECD	Organisation for Economic Co-operation and Development
P	Persistent
Pa	Pascals
PBDE	Polybromodiphenyl ether
PBT	Persistent, bioaccumulative and toxic
PCB	Polychlorinated biphenyl
POP	Persistent organic pollutant
PPB	Parts per billion
PPM	Parts per million
QSAR	Quantitative structure-activity relationship
QPREF	QSAR Prediction Reference Format
QSPR	Quantitative structure-property-relationship

r^2	Correlation coefficient
REACH	Registration, Evaluation, Authorisation and restriction of Chemicals Regulation (EC 1907/2006)
Rel.	Reliability according to the Klimisch Score
s	Seconds (time)
SIM	Selective ion monitoring
SPIN	Database of substances in products in the Nordic countries
std.dev.	Standard deviation
STOT-RE	Specific target organ toxicity – repeated exposure
SVHC	Substances of very high concern
Σ	Sum
T	Toxic (hazard classification)
US or USA	United States of America
UV	Ultraviolet
UV-234	A phenolic benzotriazole UV stabilizer, CAS 70321-86-7
UV-320	2-benzotriazol-2-yl-4,6-di-tert-butylphenol, CAS 3846-71-7
UV-326	A phenolic benzotriazole UV stabilizer, CAS 3896-11-5
UV-327	2,4-di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol, CAS 3864-99-1
UV-328	2-(2H-benzotriazol-2-yl)-4,6-ditertpentylphenol, CAS 25973-55-1
UV-329	A phenolic benzotriazole UV stabilizer, CAS 3147-75-9
UV-350	2-(2H-benzotriazol-2-yl)-4-(tert-butyl)-6-(sec-butyl)phenol, CAS 36437-37-3
UV-360	A phenolic benzotriazole UV stabilizer, CAS 103597-45-1
UV-571	A phenolic benzotriazole UV stabilizer, CAS 125304-04-3
UV-928	A phenolic benzotriazole UV stabilizer, CAS 73936-91-1
UV-P	A phenolic benzotriazole UV stabilizer, CAS 2440-22-4
vB	Very bioaccumulative
vP	Very persistent
vPvB	Very persistent, very bioaccumulative
w.a.	When applicable
ww	Wet weight
WWTP	Waste water treatment plant
YES	Yeast-estrogen-screen
YES/YAS	Yeast-Estrogen/Androgen-Screening