# 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):** **2,4-di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol (UV-327)**

**EC Number(s):** **223-383-8**

**CAS Number(s):** **3864-99-1**

**Submitted by:** **Germany**

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

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**EC Number(s): 223-383-8**

**CAS number(s): 3864-99-1**

- 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 Article 57(e) of REACH**

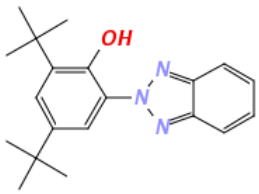
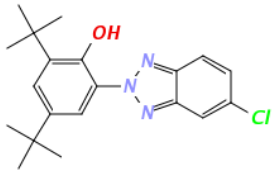
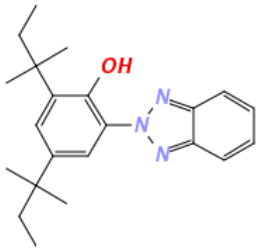
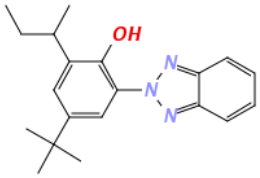
According to a Weight-of-Evidence argumentation UV-327 has to be considered vP and therefore also P. Also the substance fulfils in a MITI-study the numerical criterion to be considered vB and therefore also B. In conclusion UV-327 has vPvB-properties.

**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.

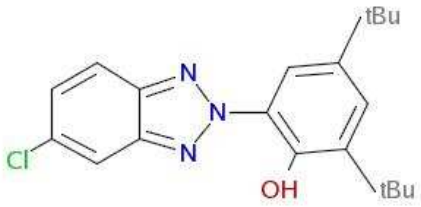
## 1.1 Name and other identifiers of the substance

**Table 2: Substance identity**

| | |
|---|---|
| EC number: | 223-383-8 |
| EC name: | 2,4-di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol |
| CAS number (in the EC inventory): | 3864-99-1 |
| CAS number: | 3864-99-1 |
| CAS name: | Phenol, 2-(5-chloro-2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)- |
| IUPAC name: | 2,4-Di-tert-butyl-6-(5-chloro-2H-benzotriazol-2-yl)phenol |
| Index number in Annex VI of the CLP Regulation | - |
| Molecular formula: | C20H24ClN3O |
| Molecular weight range: | 357.8771 g/mol |
| Synonyms: | Phenol, 2,4-di-tert-butyl-6-(5-chloro-2H-benzotriazol-2-yl)-;<br>2,4-Di-tert-butyl-6-(5-chloro-2H-benzotriazol-2-yl)phenol;<br>2,4-di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol;<br>2-(2-Hydroxy-3,5-di-tert-butylphenyl)-5-chloro-2H-benzotriazole;<br>2-(2-Hydroxy-3,5-di-tert-butylphenyl)-5-chlorobenzotriazole;<br>2-(2'-Hydroxy-3',5'-di-tert-butylphenyl)-5-chlorobenzotriazole;<br>2-(3,5-Di-tert-butyl-2-hydroxyphenyl)-5-chloro-2H-benzotriazole;<br>2-(3,5-Di-tert-butyl-2-hydroxyphenyl)-5-chlorobenzotriazole;<br>2-(3',5'-Di-tert-butyl-2'-hydroxyphenyl)-5-chlorobenzotriazole;<br>5-Chloro-2-(2-hydroxy-3,5-di-tert-butylphenyl)-2H-benzotriazole;<br>5-Chloro-2-(2-hydroxy-3,5-di-tert-butylphenyl)benzotriazole;<br>5-Chloro-2-(3,5-di-tert-butyl-2-hydroxyphenyl)-2H-benzotriazole;<br>5-Chloro-2-(3,5-di-tert-butyl-2-hydroxyphenyl)benzotriazole;<br>5-Chloro-2-(3',5'-di-tert-butyl-2'-hydroxyphenyl)benzotriazole;<br>ADK Stab LA 34;<br>Antioxidant 327;<br>Cyasorb UV 5357;<br>Eversorb 75;<br>Hisorb 327;<br>Hisorp 327; |

| | |
|---|---|
| | Kemisorb 72;<br>LA 34;<br>Lowilite 27;<br>Mark LA 34;<br>Seesorb 702;<br>TNV 327;<br>Tinuvin 327;<br>UV 2;<br>UV 2 (UV stabilizer);<br>UV-327;<br>UV-Chek AM 607;<br>Viosorb 580 |

**Structural formula:**




## 1.2 Composition of the substance

**Name: 2,4-di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol**

**Description: mono-constituent**

**Degree of purity: >=98%[1]**

**Table 3: Constituents**

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

[1] From C&L notifications

| Constituents | Typical concentration | Concentration range | Remarks |
|---|---|---|---|
| 2,4-di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol<br>EC-number: 223-383-8 | | | |

**Table 4: Impurities**

| Impurities | Typical concentration | Concentration range | Remarks |
|---|---|---|---|
| *n.a.* | | | |

**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 | 154 - 156 °C | Rosevear, Judi; Australian Journal of Chemistry, V38(8). P1163-76 |
| Boiling point | 469.2±55.0 °C | Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs) |
| Vapour pressure | $2.00E^{-9}$ Torr | Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 A |
| Water solubility | 0.026 mg/l | result from WSkowWIN v1.42; US EPA 2011 |
| Partition coefficient n-octanol/water (log value) | 7.544 ± 1.258<br>6.91<br>7.91 | Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs)<br>EPISuite v.4.10<br>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. Therefore the self classifications according to Regulation 1272/2008/EC (CLP) from ECHA's C&L Inventory database (accessed 09.10.2012) 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 expected to withstand hydrolysis 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-327.

#### 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 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 9.749 hours, the overall OH-rate constant was estimated to be $1.32*10^{-11}$ 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-327 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-327 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-327 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-327 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-327 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 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

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

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 break down of the phenolic benzotriazole moiety begins only when two vicinal hydroxyl groups on the phenolic 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.

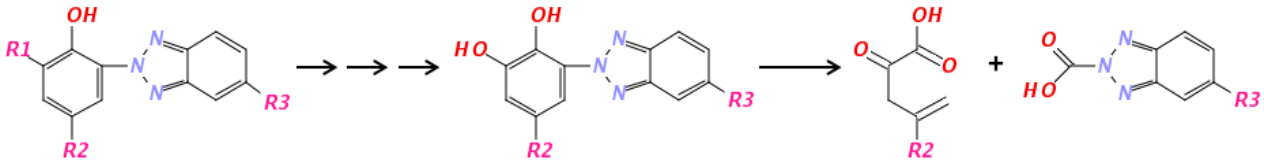



**Figure 1: Proposed mechanism for the ring cleavage of the phenolic moiety of the phenolic benzotriazoles, R1: H, alkyl, aryl or alkyl-aryl; R2: alkyl, aryl or alkyl-aryl; R3: H or Cl. Side reactions are for the sake of simplicity not considered here.**

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 degraded stepwise. In case of UV-327 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 0.0013 indicating that the substance does not biodegrade fast.
- Biowin6 (MITI non-linear biodegradation probability) results in a value of 0.0024 indicating that the substance is not readily degradable.
- Biowin3 (Survey model – ultimate biodegradation) results in a value of 1.8338 indicating that the degradation will take more than a month.

#### 3.1.2.1.2 Screening tests

In a 14 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 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.

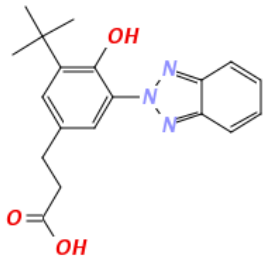



**Figure 2: M1 (CAS 84268-36-0) is the first metabolite of degradation of EC 407-000-3**

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 72 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.

#### 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-327 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. 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 degradation 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-327, 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-327, if there is degradation.

In addition to the studies described above, there is a case of monitoring studies that shows that the substance is not completely degraded in sediments even after decades. UV-327 was produced in an American specialty chemicals manufacturing plant near the Pawtuxet River between 1963 and 1972 (Jungclaus et al., 1978); (Lopez-Avila and Hites, 1980), (Reddy et al., 2000a)). Sediment samples were taken 4 years after production of UV-327 stopped and the substance was still detected at concentrations of 2 - 300 ppm (Jungclaus et al., 1978). Lopez-Avila and Hites (1980) report sediment concentrations of 300 and 400 ppm near the plant, 20 and 80 ppm towards the mouth of the Pawtuxet River and further decreasing concentrations in the subsequent Providence River with increasing distance from the point of discharge. The Providence River empties into Narragansett Bay. One sediment core from the Pawtuxet River (from 1989) and one from Narragansett Bay (from 1997) were sectioned and analyzed (Reddy et al., 2000). In the Pawtuxet River core UV-327 was

detected in concentrations up to ca. 5 mg/g (17 years after production stop). In the Narragansett Bay core the maximum concentration of UV-327 was ca. 25 µg/g (25 years after production stop). Hartmann et al. (2005) analyzed more sediment cores from Narragansett Bay. Cores were taken 25 years after production of UV-327 stopped. The highest concentration of UV-327 was ca. 690 ng/g dw in a core section taken at 40 – 50 cm depth. The authors use UV-327 as a tracer, because it is known when production of the substance started and when it was discontinued. A sharp rise of the UV-327 concentration in the sediment core indicates the introduction of UV-327. Production of UV-328 started and stopped later than production of UV-327 at the same location, therefore the ratio of UV-327 to UV-328 concentrations in the sediment is also used for tracing sediment deposition processes. This case shows that UV-327 is indeed very slowly degraded in sediment.

Sediment concentrations in the range of µg/g dw were also found in Sweden (Brorström-Lundén et al., 2011). In Sweden 18 µg/g dw were also measured at a background site. . 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 at background sites. The authors do not offer an explanation for this. It should also be noted that the detection limits for sediments were very high in the Swedish study.

The overall evidence presented in chapter 3.1.2 in combination with the high-potential for adsorption on soil and suspended organic matter and the degradation behaviour of UV-327 in the sediments of the Pawtuxet River indicate in a Weight-of-Evidence approach that UV-327 will be persistent in the environment.

This is supported by numerous findings of UV-327 in the environment (see part II). UV-327 was frequently investigated in monitoring studies. Studies are available from Sweden, Germany, Spain (and Portugal), USA, the Philippines, China and Japan (with certain data from other Asian countries and Poland). The substance was frequently detected in air, air deposition, dust from houses, roads and car cabins, in soil, surface water, sediments, aquatic organisms, water fowl, marine mammals, in WWTP influent, effluent and sludge, in storm water, landfill effluent, foodstuff and human adipose tissue. The measured concentrations show a widespread contamination of the environment over all compartments with highest concentrations in dust, (soil), sediments, biota (based on lipid weight) and WWTP sludge. In Japan an increasing trend of UV-327 concentrations in marine sediments was ascertained by Nakata et al. (2011) after investigations of sediment cores.

## 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. Details of the prediction can be found in Annex 3. The default input parameters were used.

**Table 9: Results adsorption behaviour predictions of UV-327**

| Model | QSAR result | Overall model performance | QPREF |
|---|---|---|---|
| EPISuite 4.1 KOW-method | $K_{OC}$ (L/kg): 1.91 $10^5$<br>Log $K_{OC}$: 4.99 | Reliable with Restrictions | Annex 3.4 |
| EPISuite 4.1 MCI-method | $K_{OC}$ (L/kg): 9.77 $10^4$<br>Log $K_{OC}$: 5.28 | Reliable with Restrictions | Annex 3.4 |
| COSMOtherm | $K_{OC}$ (L/kg): 4.57 $10^5$<br>Log $K_{OC}$: 5.66 | Reliable with Restrictions | Annex 3.4 |

The results of the estimation of the adsorption behaviour lead to the conclusion that UV-327 will strongly adsorb to organic material.

### 3.2.2 Volatilisation

The tendency for volatilization from the water phase was estimated by calculation of the Henry constant. Using the physical-chemical substance properties from Table 6 and a water solubility of 0.026 mg/l (result from WSkowWIN v1.42; US EPA 2011), the calculated Henry constant[3] was determined to be $4.337*10^{-3}$ Pa*m³*Mol-1, indicating only little tendency for volatilization. The air-water partitioning coefficient (Kair-water) may be derived from the Henry's law constant and is calculated to be $1.78*10^{-6}$ m3/m3. The Kair-water and Henry's law constant are very low suggesting that volatilisation is unlikely to be a significant removal mechanism for UV-327 from aquatic systems and it is unlikely that the substance will be transported very far in the atmosphere (based on its atmospheric half-life estimated to be 9.749 hours).

### 3.2.3 Distribution modelling

*Fugacity Level III distribution modelling*

When released to the environment UV-327 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)

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

| Compartment | mass amount (percent) |
|---|---|
| Air | $5.39*10^{-5}$ |
| water | 3.96 |
| soil | 60.7 |
| sediment | 35.4 |

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 (60.7 %) and the sediment (35.4%).

***Distribution in waste water treatment plants***

The dominant route of exposure for UV-327 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 readily biodegradable (k=0/h). The substance properties were taken from Table 6 except of the water solubility of 0.026 mg/l which was calculated with WSkowWIN v1.42.

**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 | 8.7 |
| via primary sludge | 66.2 |
| via surplus sludge | 25.1 |
| degraded | 0.0 |
| *total* | *100* |

The results of the calculation lead to the conclusion that when UV-327 is released into waste water the largest part of the substance will be hold 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 purposes 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-327. 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-327**

| Model | QSAR result | Overall model performance | QPREF |
|---|---|---|---|
| EPISuite 4.1 KOWWIN | Log $K_{OW}$: 6.91 | Reliable | Annex 4.3 |
| COSMOtherm | Log $K_{OW}$: 7.91 | Reliable | Annex 4.3 |

Based on the estimated log $K_{OW}$-values that are larger than 4.5, it is expected that UV-327 will bioaccumulate.

### 3.3.1 Aquatic bioaccumulation

UV-327 was tested in two bioconcentration studies according to OECD 305 C (NITE, 2012; reliability rated Klimisch 2). Not all test conditions can be reported because the summary of the studies does not list them. Three different substance concentrations were tested in common carp (Cyprinus carpio) in the tests. The test conditions are given in Table 13. Since UV-327 has a low water-solubility dispersants were used.

**Table 13: Test conditions of the two bioconcentration studies.**

| Test concentration in µg/L | duration | Dispersant used |
|---|---|---|
| 1.0 | 60 | HCO-20: 20µg/L and olive oil: 10µg/L |
| 0.1 | 68 | HCO-20: 2µg/L and olive oil: 1µg/L |
| 0.1 | 60 | N,N-zdimethylformamide: 47000 µg/L |
| 0.01 | 60 | N,N-zdimethylformamide: 47000 µg/L |

Table 14 lists the original report data amended with the BCF normalised to 5 % lipid content. Calculations were done with the average of the reported lipid content of fish at start and end of the test.

**Table 14: BCF reported** and **BCF lipid normalised of UV-327 (values refer to whole body wet weight basis unless no other information is provided)**

| Test concentration in µg/L | $BCF_{reported}$ | $BCF_{lipid\text{-}normalised}$ |
|---|---|---|
| 1.0 | 900[1] | 1203 |
| 0.1 | 4700[1] | 6283 |
| 0.1 | 7600[2] | 8817 |
| 0.01 | 6500[2] | 7540 |

[1] Average lipid content of test fish 3.74 %

[2] Average lipid content of test fish 4.31 %

Lowest BCF values were found for the highest test concentration. This may be ascribed to test concentration being near to water solubility which frequently results in impaired accuracy of analysis. The majority of lipid normalised BCF values are well above the vB-criterion. Only at the highest test concentration of 1 µg/L the vB-criterion is not met and neither is the B-criterion.

Nakata et al (Nakata et al., 2010) studied occurrence of several benzotriazoles in blubber of finless porpoise (*Neophocaena phocaenoides*) of the Ariake Sea. They report a BAF of 33300 for UV-327 as an average of 5 Individuals sampled from 1998 to 2009. The authors recalculated this value from blubber concentration to whole body using an empirical average lipid content of finless porpoises of 28 %. This equates to a BAF of 5946 for 5 % lipid content. The study has some deficiencies, e.g. a long time period over which the samples were taken. Also only a low number of samples were available and a recalculation to whole body was necessary which is not uncommon in case of mammalian samples in monitoring studies. Some further aspects should be considered when evaluating the study. The Ariake Sea is a large bay with a maximum depth of 50 meters. Such shallow depths are preferred by finless porpoises. The bay is surrounded by several cities, e.g. Nagasaki. Therefore it is probable that there has been a steady exposition to phenolic benzotriazoles in this region in recent years. Monitoring studies confirm this assumption (*cf.* Annex 5). As phenolic benzotriazoles adsorb strongly to suspended matter and sediment it is probable that the entry path into the food chain are benthic animal taking up UV-327 from sediment. Considering nutrition behaviour of finless porpoises and its prey creates a plausible picture of transport of UV-327 through the food chain. Finless porpoises feed on small fish but also on shrimps and cephalopods, e.g. squids. Squids are carnivorous and feed on fish but also on crabs which are benthic omnivores, feeding e.g. on carrion. Shrimps feed on detritus and algae which have a large adsorption surface and are known to have weak elimination capabilities. Finless porpoises of this region also feed on sand eels (*Amodytes tobianus*) which again feed on crabs and cephalopods. Thus it is probable that finless porpoise accumulated UV-327 by food. The determined bioaccumulation factor clearly is above the trigger value for vB. UV-327 enriches in top predators.

### 3.3.2 Terrestrial bioaccumulation

No data available.

### 3.3.3 Summary and discussion of bioaccumulation

With exception of the highest test concentration all results show that UV-327 meets the vB-criterion BCF. Additionally, a lipid-normalised field BAF of 5946 for UV-327 was found in a monitoring study by Nakata (Nakata et al., 2010).

There are biomonitoring studies that suggest a strong dependency of the bioaccumulation potential of phenolic benzotriazoles on the species considered. Enrichment in top predators is at least in some cases suggested (see Annex 5).

The bioaccumulative characteristics of UV-327 are supported by numerous findings of the substance in aquatic biota in monitoring studies. In marine fish and marine tidal flat organisms concentrations of more than one hundred ng/g lw were found (Kim et al., 2011 b and c; Nakata et al., 2009a). In mussels such high concentrations were found regularly (Nakata et al., 2012). Concentrations were lower, but still regularly found in marine shallow water organisms (Nakata et al., 2009a) and in human adipose tissue (Yanagimoto et al., 2011). UV-327 is accumulated in the blubber of marine mammals and an increasing temporal trend is stated for marine mammals in Japan (Nakata, 2011).

In Sweden concentrations in fish in the µg/g dw range were reported, even in samples from background sites (Brorström-Lundén et al., 2011). On the other hand the Swedish study is the only

one with measured concentrations of that level. The authors do not offer an explanation for this. It should also be noted that the detection limits for biota were very high in the Swedish study.

In summary monitoring data on UV-327 can give a certain indication that bioaccumulation may occur.

Structural similar substances confirm the overall assessment. UV-320 (CAS 3846-71-7) and UV-350 (CAS 36437-37-3) have been shown to meet the vB-criterion as well. Furthermore, data for structural similar substances support the conclusion as well. Table 15 gives an overview over the available data on bioconcentration on all four phenolic benzotraizoles discussed.

**Table 15: 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

## 3.4 Secondary poisoning

UV-327 and UV-328 enrich in top predators (*cf.* 3.3.1). A lipid-normalised BAF of 5946 was found in finless porpoise. Though no direct proof was given in the study itself the habitat may be assumed as having been continuously exposed to phenolic benzotriazoles and such has been the prey. Several biomonitoring studies suggest that as well (see Annex 5). Moreover, adsorptivity of UV-327 and information on the diet of finless porpoise and its prey show a plausible and very probable transport of the substance through the food chain. Thus it is concluded that UV-327 accumulates through the food chain. This is supported to some extent by the appearance of the substance in foodstuff and (in

higher concentrations) in human adipose tissue (Yanagimoto et al., 2011). However, uptake by humans could also take place via air, dust etc.

# 4 HUMAN HEALTH HAZARD ASSESSMENT

Not relevant for this dossier.

# 5 ENVIRONMENTAL HAZARD ASSESSMENT

## 5.1 Aquatic compartment (including sediment)

### 5.1.1 Toxicity data

#### 5.1.1.1 Fish

##### 5.1.1.1.1 Short-term toxicity to fish

In 2004 a study was presented under the Existing Chemicals Law of Japan were in a 96 h acute toxicity test a $LC_{50}$ of >25 mg $l^{-1}$ was reported, meaning no effect was found until the water solubility limit was reached. Not all test conditions can be reported because not all text passages could be translated as the original report is available in Japanese, only.

**Table 16: Acute toxicity of UV-327 on fish.**

| Species | Duration | $LC_{50}$ (mg $l^{-1}$) | Method, conditions | Rel. | Reference |
|---|---|---|---|---|---|
| *Oryzias latipes* | 96 h | >25 | Japanese Industrial Standard (JIS K 0102-1998-71.), "Testing methods for industrial waste water, Acute toxicity test with fish | 2 | (Japan, 2004) |

##### 5.1.1.1.2 Long-term toxicity to fish

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

#### 5.1.1.2 Aquatic invertebrates

##### 5.1.1.2.1 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* at concentrations 0.1, 0.5, 1.0, 5.0 and 10.0 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-327 on aquatic invertebrates.

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

#### 5.1.1.2.2 Long-term toxicity to aquatic invertebrates

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

### 5.1.1.3 Algae and aquatic plants

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

### 5.1.1.4 Sediment organisms

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

### 5.1.1.5 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 in literature 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-327 is degraded, biodegradation is expected to be the most relevant pathway for degradation . Although there are no simulation tests on UV-327 itself, based on a Weight-of-Evidence Argumentation it can be shown that UV-327 is very persistent. This argumentation is based on the following facts;

- In many environmental monitoring studies UV-327 is analysed in a variety of different compartments in many regions of the world. Of special importance is the case of several studies on sediments of the Pawtuxet River, where UV-327 is found in deeper sediments even decades after the production of this substance in a nearby chemical plant has stopped.
- Once released into the environment most UV-327 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-327 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 exists 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 we therefore assess that UV-327 must be considered to be very persistent in the environment.

#### 6.1.1.2 Bioaccumulation

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

#### 6.1.1.3 Toxicity

The available studies show that UV-327 is not acutely toxic for aquatic organisms. There is no information on the long-term toxicity of UV-327. Based on the currently available data we conclude that UV-327 does not fulfil the T-criterion.

### 6.1.2 Summary and overall conclusions on the PBT, vPvB properties

UV-327 has to be considered vP and P. Also the substance fulfils the numerical criterion to be considered vB and B. In conclusion UV-327 has vPvB- 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 –CONCLUSIONS ON EXPOSURE

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). Besides the group of benzophenones they are technically the most important UV-absorbers, especially for transparent plastic materials. The different phenolic benzotriazoles have different substitution patterna 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.

The number of individual notifications in ECHA's C&L Inventory database[4] (total number: 418, subdivided into 20 different aggregated notifications) leads to the conclusion that UV-327 is commercially relevant within Europe.

Concerning tonnages manufactured or imported we do not have a complete picture of the situation yet, as UV-327 is not registered under REACH in the moment. The substance is contained in the ECHA list on "Substances Identified for 2013 Registration" - therefore and because of the high number of notifications in the C&L Inventory database several registration dossiers in the band of 100 – 1000 tonnes per year are expected. It has to be kept in mind that the dossiers only cover a single registrant. Even when only a handful of the 20 aggregated notifiers of the C&L inventory might submit a registration dossier for a tonnage band of 100 – 1000 tonnes per year the aggregated tonnages over all registrants might exceed threshold of 1000 tonnes per year without circumstances.

We contacted EUROSTAT to get data on the import and export of phenolic benzotriazoles. Only for UV-327 data is explicitly available. These data is presented in Table 1818.

[4] http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database; (accessed 19. Febraury 2013)

**Table 18: Import and Export of UV-327 in the EU27**

| | **2006** | **2007** | **2008** | **2009** | **2010** |
|---|---|---|---|---|---|
| Import into EU 27 | 287.7 | 193.3 | 145.2 | 64.3 | 59.8 |
| Export out of EU 27[5] | 32.3 | 43.1 | 125.5 | 8084[6] | 890.1 |

From this import-export data acquired from EUROSTAT and the high number of notifications in ECHA's C&L Inventory it can be assumed that UV-327 will be registered in 2013 as well. The substance is also on ECHA´s list of substances to be registered in 2013.

According to our general knowledge on phenolic benzotriazoles, we expect that UV-327 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[7] (SPIN) refers to 100 preparations from Sweden, Denmark, Finland and Norway which contain UV-327 and to some extent these preparations are sold to consumers. The information on used quantities specifies 1.4 tonnes UV-327 being supplied in preparations per year in Denmark and 1.0 tonnes in Sweden (reporting year: 2010 each). Norway and Finland only reported a tonnage of 0.0 tonnes for 2010, with a low number of only 8 respectively 4 preparations put on the market in those two countries.

**Measured environmental concentrations**

UV-327 was detected in six of eight air samples (0.40 – 25 ng/m³) and three of four air deposition samples (<100 – 320 ng/m² day) in Sweden (Brorström-Lundén et al., 2011).

In house dust from private houses in Spain UV-327 was detected in all 5 analyzed samples in concentrations of 22 – 101 ng/g (Carpinteiro et al., 2010a). In a public building the concentration was 131 ng/g, in 3 car cabins 43 – 127 ng/g and in a dust reference material from the USA 322 ng/g. UV-327 was detected in 88% of 37 house dust samples from Manila (Kim et al., 2012). The median concentration in dust from a residential area was 19 ng/g, the maximum 73 ng/g. UV-327 was also detected in road dust in Japan with concentrations from ca. 8 to 116.9 ng/g dw (Nakata et al., 2011).

Three Swedish soil samples contained UV-327 in concentrations from 0.6 to 3.7 µg/g dw (Brorström-Lundén et al., 2011). In Germany UV-327 was not detected in 3 soils with high anthropogenic influence and 2 soils from background sites (Rodríguez Pereiro and Casado Agrelo, 2012).

[5] almost exclusively from UK

[6] Please note: We do not know if the export peak in 2009 is an error due to a misplaced comma, but expect it to be.

[7] Information from SPIN-database (www.spin2000.net; accessed 24.07.2012)

In four of six surface water samples of Sweden UV-327 was present at low concentrations (0.11-0.39 ng/L) (Brorström-Lundén et al., 2011).Two of these four samples were from background sites. The substance was not found in three samples of river water and in 12 seawater samples from Spain ( (Carpinteiro et al., 2010b). (Montesdeoca-Esponda et al., 2012)). UV-327 was detected in 8 of 20 surface water samples (rivers, streams, lakes) in Japan with concentrations from 1 – 6 ng/L (Kameda et al., 2011). It was not found in water samples from background sites.

In Germany UV-327 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).

Brorström-Lundén et al. (2011) found UV-327 in all six sediments investigated, including background sites. Concentrations were much higher than in other countries and ranged from 1.6 to 35 µg/g dw. Carpinteiro et al. (Carpinteiro et al., 2012a) detected UV-327 in 3 of 10 European sediments at concentrations of 9.5 - 15 ng/g. In marine and estuarine sediments in Japan (n = 11) UV-327 was present in concentrations ranging from 1.6 to 9.9 ng/g dw, in five samples of polluted river sediments concentrations were 16 – 190 ng/g dw (Nakata et al., 2009a). In 21 of 24 sediment samples from Japan UV-327 was detected in concentrations ranging from 0.4 – 37 ng/g dw (Kameda et al., 2011).Sediment samples from background sites still showed UV-327 concentrations of up to 1.1 ng/g dw. UV-327 was significantly correlated with sediment concentrations of HHCB, an indicator chemical for domestic wastewaters and WWTP effluents. UV-327 was detected in one of six sediment samples from a Chinese River (0.310 ng/g dw) and in three of six sediment samples from two rivers in the U.S. (0.22-1.90 ng/g dw) (Zhang et al., 2011). Investigation of 2 sediment cores from Japan showed an increasing temporal trend for UV-327 (Nakata et al., 2011). Concentrations start to rise around 1970, highest concentrations were ca. 4 and ca. 8 ng/g dw, respectively.

UV-327 was neither detected in treated industrial wastewater of an American specialty chemicals manufacturing plant, nor in the receiving Pawtuxet River water ((Jungclaus et al., 1978); (Lopez-Avila and Hites, 1980)). UV-327 was manufactured at the plant between 1963 and 1972. Sediment samples were taken 4 years after production of UV-327 stopped and the substance was still detected at concentrations of 2 - 300 ppm (Jungclaus et al., 1978) Lopez-Avila and Hites (1980) report sediment concentrations of 300 and 400 ppm near the plant, 20 and 80 ppm towards the mouth of the Pawtuxet River and further decreasing concentrations in the subsequent Providence River with increasing distance from the point of discharge. The Providence River empties into Narragansett Bay. Hard shell clam tissue from Narragansett Bay showed higher UV-327 concentrations (1.0 – 8.5 ng/g ww) than tissue from a control location (Pruell et al., 1984). One sediment core from the Pawtuxet River (from 1989) and one from Narragansett Bay (from 1997) were sectioned and analyzed (Reddy et al., 2000a). In the Pawtuxet River core UV-327 was detected in concentrations up to ca. 5 mg/g (17 years after production stop). In the Narragansett Bay core the maximum concentration of UV-327 was ca. 25 µg/g (25 years after production stop). Further investigations of sediment cores taken in 1997 showed UV-327 concentrations of up to ca. 690 ng/g dw in certain sections (Hartmann et al., 2005).

In Sweden UV-327 was present in three of four fish samples (2.3 – 9.8 µg/g dw) (Brorström-Lundén et al., 2011). In 8 of 10 species of marine tidal flat organisms from Japan (n = 19) UV-327 was present at concentrations of 0.62 – 3.6 ng/g ww (Nakata et al., 2009a). Based on lipid weight highest concentrations were found in tidal flat clam, crab and herbivorous mudskipper (> 100 ng/g lw). In 9 of 10 species of marine shallow water organisms (n = 18) concentrations were lower (0.29 – 2.3 ng/g ww), whereas in the liver of 6 species of shallow water organisms (n = 13) higher concentrations were detected (2.4 – 13 ng/g ww). In the liver of spot-billed duck and mallard concentrations were 2.6 and 3.4 ng/g ww (90 and 59 ng/g lw, respectively). A further study on

marine organisms from Japan confirms that UV-327 is especially found in lipid of lower benthic organisms collected from tidal flat areas and in the liver of water fowl (Nakata et al., 2009b). UV-327 was detected in blue and green mussels in 6 of 10 Asian countries with highest concentrations in Hong Kong and Korea (ca. 0.3 µg/g lw) ((Nakata, 2011); (Nakata et al., 2012)). In mussels from the U.S. west coast UV-327 was detected in 11 of 15 samples and concentrations were similar (Nakata et al., 2012). UV-327 was detected in 5 samples of the blubber of finless porpoises in Japan in concentrations ranging from 4.5 to 31 ng/g ww (Nakata et al., 2010). UV-327 was not detected in blubber samples of marine mammals from around 1980, but in samples taken in 1990 and later (increasing trend, n = 33) (Nakata et al., 2011). The maximum concentration was ca. 45 ng/g lw. In fish muscle samples from the Philippines (3 species, n = 5) UV-327 was present in concentrations ranging from 2.57 to 18.5 ng/g lw (Kim et al., 2011b). In a further study on 20 species (n = 58) UV-327 was detected in 43% of the samples. Concentrations ranged from n.d. to 221 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.

Brorström-Lundén et al. (2011) found UV-327 in four of five WWTP effluents (0.12 – 0.48 ng/L), in particles of a WWTP effluent (270 µg/g dw) and in seven of eight WWTP sludges (0.54 - 17 µg/g dw.). UV-327 was not detected in raw and treated wastewater in Spain (Carpinteiro et al., 2010b). In another study it was detected in raw wastewater of 1 of 2 Spanish WWTPs (22 ng/L) and in raw wastewater of a Portuguese WWTP (85 ng/L) (Carpinteiro et al., 2012b). It was present in treated wastewater of the Portuguese WWTP (31 ng/L), but not in treated wastewater of both Spanish WWTPs. Montesdeoca-Esponda et al. (2012) found UV-327 in one of seven Spanish WWTP effluents at a concentration of 4.8 ng/L. In Japan UV-327 was detected in 1 of 4 WWTP effluents (2 ng/L) (Kameda et al., 2011). In water samples from the influent of five WWTPs in Japan UV-327 was present at concentrations of 9.2 and 12 ng/L, whereas the effluents all contained < 8.7 ng/L (Nakata and Shinohara, 2010). In sludge 120 – 200 ng/g dw were measured. Zhang et al. (2011) detected UV-327 in four of five sewage sludge samples from Chinese WWTPs (1.80-8.40 ng/g dw). Ruan et al. (Ruan et al., 2012) found 1.53 – 133 ng/g dw in 24 of 60 sewage sludge samples from Chinese municipal WWTPs (median 14 ng/g dw).

In Sweden Brorström-Lundèn found UV-327 in two of three landfill effluents (0.45 and 1.3 ng/L), in one sample of landfill effluent particles (4.3µg/g dw) and three of four storm water samples (0.13 – 0.17 ng/L).

Concentration of UV-327 in “refuse derived fuels” obtained from Japanese municipal solid waste after removing the incombustible materials was 20 ng/g (Watanabe and Noma, 2010). After treatment in a pilot-scale incinerator the concentration in the flue gas (final exit) was 0.0042 µg/m³. Bottom ash contained 0.063 ng/g UV-327, fly ash 0.049 ng/g.

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 (Yanagimoto et al., 2011). Lowest concentrations were observed in the USA (up to ca. 5 ng/g lw). In foodstuff highest UV-327 concentrations were detected in seafood (up to ca. 1.4 ng/g ww) and meat (up to ca. 1.2 ng/g ww). Meat with high concentrations was imported from the USA and Australia. Lower concentrations were detected in vegetables (up to ca. 0.3 ng/g ww) and some fruit (up to ca. 0.5 ng/g ww). In dairy products no benzotriazole UV stabilizers were found.

**Table 19: Overview of UV-327 concentrations in the environment**

| Compartment | Concentration | Detection frequency* | Country of sampling | Reference |
|---|---|---|---|---|
| air | 0.57 - 25 ng/m³<br>background sites:<br>0.40 and 9.2 ng/m³ | 4/6<br><br>2/2 | Sweden | (Brorström-Lundén et al., 2011) |
| air deposition | 234 and 303 ng/m² day<br>background sites: 318 ng/m² day | 2/2<br><br>1/2 | Sweden | (Brorström-Lundén et al., 2011) |
| dust | median 19 ng/g<br>max. 73 ng/g<br>(residential area) | 33/37 | Philippines | (Kim et al., 2012) |
| | 22 – 101 ng/g (private houses)<br>131 ng/g<br>(public building)<br>43 – 127 ng/g<br>(car cabins) | 5/5<br><br>1/1<br><br>3/3 | Spain | (Carpinteiro et al., 2010a) |
| | 322 ng/g (dust reference material) | 1/1 | USA | (Carpinteiro et al., 2010a) |
| road dust | ca. 8 - ca. 116.9 ng/g dw | 9/9 | Japan | (Nakata et al., 2011) |
| soil | 0.66 - 3.7 µg/g dw<br>background site: n.d. | 3/3<br>0/1 | 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 | 0.26 and 0.39 ng/L<br>background sites: 0.11 and 0.13 ng/L | 2/4<br><br>2/2 | Sweden | (Brorström-Lundén et al., 2011) |
| | 1 – 6 ng/L<br>background sites: n.d. | 8/20<br><br>0/5 | Japan | (Kameda et al., 2011). |
| | n.d. | 0/3 | Spain | (Carpinteiro et al., 2010b) |
| | n.d.<br>(industrial pollution) | 0/16 | USA | (Jungclaus et al., 1978) |
| | n.d.<br>(industrial pollution) | 0/25 | USA | (Lopez-Avila and Hites, 1980) |
| suspended solids (from river water) | n.d. (background sites, sites with high anthropogenic influence) | 0/5 | Germany | (Rodríguez Pereiro and Casado Agrelo, 2012) |

| | | | | |
|---|---|---|---|---|
| seawater | n.d. | 0/12 | Spain | (Montesdeoca-Esponda et al., 2012) |
| sediment | 1.6 – 35 µg/g dw<br>background sites:<br>1.6 – 18 µg/g dw | 3/3<br><br>3/3 | Sweden | (Brorström-Lundén et al., 2011) |
| | 0.31 ng/g dw | 1/6 | China | (Zhang et al., 2011) |
| | 0.22 – 1.90 ng/g dw | 3/6 | USA | |
| | max. ca. 5 mg/g (core, industrial pollution) | 2/2 | USA | (Reddy et al., 2000a) |
| | max. ca. 690 ng/g dw (core, industrial pollution) | 3/3 | USA | (Hartmann et al., 2005) |
| | 2 – 300 ppm (industrial pollution) | ?/19 | USA | (Jungclaus et al., 1978) |
| | max. 400 ppm (industrial pollution) | 25/25? | USA | (Lopez-Avila and Hites, 1980) |
| | 9.5 – 15 ng/g | 3/10 | Europe | (Carpinteiro et al., 2012a) |
| | 16 – 190 ng/g dw<br>(polluted river) | 5/5 | Japan | (Nakata et al., 2009a) |
| | 0.3 – 37 ng/g dw<br>background sites:<br>0.5 – 1.1 ng/g dw | 21/24<br>2/5 | Japan | (Kameda et al., 2011). |
| marine sediment | 1.6 – 9.9 ng/g dw | 11/11 | Japan | (Nakata et al., 2009a) |
| | max. ca. 4 and ca. 8 ng/g dw (2 cores, increasing trend) | 2/2 | Japan | (Nakata et al., 2011) |
| fish | 4 µg/g dw<br>background sites:<br>2.3 and 9.8 µg/g dw | 1/2<br><br>2/2 | Sweden | (Brorström-Lundén et al., 2011) |
| marine fish | 2.57 – 18.5 ng/g lw | 5/5 | Philippines | (Kim et al., 2011b) |
| | max. 221 ng/g lw | 25/58 | Philippines | (Kim et al., 2011c) |
| marine tidal flat organisms (incl. fish) | 0.62 – 3.6 ng/g ww<br>max. > 100 ng/g lw | 8/10 species | Japan | (Nakata et al., 2009a) |
| mussels | 61 – 280 ng/g lw<br>mean 100 ng/g lw<br>geometric mean 56 ng/g lw | 11/17 | Korea | (Nakata et al., 2012) |
| | 23 - 300 ng/g lw<br>mean 93 ng/g lw<br>geometric mean 48 ng/g lw | 6/8 | Hong Kong | |
| | 34 -150 ng/g lw<br>mean 38 ng/g lw<br>geometric mean 15 ng/g | 3/7 | Japan | |

| | | | | |
|---|---|---|---|---|
| | lw | | | |
| | 45 – 160 ng/g lw<br>mean 84 ng/g lw<br>geometric mean 65 ng/g lw | 4/5 | China | |
| | 120 and 180 ng/g lw<br>mean 150 ng/g lw<br>geometric mean 150 ng/g lw | 2/2 | Philippines | |
| | 21 and 94 ng/g lw<br>mean 58 ng/g lw<br>geometric mean 45 ng/g lw | 2/2 | Indonesia | |
| | n.d. | 0/4 | Malaysia | |
| | n.d. | 0/3 | Vietnam | |
| | n.d. | 0/3 | India | |
| | n.d. | 0/2 | Cambodia | |
| | 33 – 220 ng/g lw<br>mean 61 ng/g lw<br>geometric mean 45 ng/g lw | 11/17 | USA | |
| marine shallow water organisms (incl. fish) | 9 species:<br>0.29 – 2.3 ng/g ww<br>6 species in liver:<br>2.4 – 13 ng/g ww | 15/16 species | Japan | (Nakata et al., 2009a) |
| water fowl | liver:<br>2.6 and 3.4 ng/g ww<br>(90 and 59 ng/g lw) | 2/2 species | Japan | |
| marine mammals | blubber:<br>4.5 - 31 ng/g ww | 5/5 | Japan | (Nakata et al., 2010) |
| | blubber:<br>max. 45 ng/g lw<br>(increasing trend) | 23/32 | Japan | (Nakata et al., 2011) |
| wastewater | 85 ng/L<br>22 ng/L | 1/1<br>1/2 | Portugal<br>Spain | (Carpinteiro et al., 2012b) |
| | n.d. | 0/5 | Spain | (Carpinteiro et al., 2010b) |
| | 9.2 and 12 ng/L | 2/5 | Japan | (Nakata and Shinohara, 2010) |
| WWTP effluent | 31 ng/L<br>n.d. | 1/1<br>0/2 | Portugal<br>Spain | (Carpinteiro et al., 2012b) |
| | n.d. | 0/1 | Spain | (Carpinteiro et al., 2010b) |
| | 4.8 ng/L | 1/7 | Spain | (Montesdeoca-Esponda et al., 2012) |

| | | | | | |
|---|---|---|---|---|---|
| | | 0.12 – 0.48 ng/L<br>particles:<br>270 µg/g dw | 4/5<br><br>1/1 | Sweden | (Brorström-Lundén et al., 2011) |
| | | n.d.<br>(industrial WWTP) | ? | USA | (Jungclaus et al., 1978) |
| | | n.d. | 0/5 | Japan | (Nakata and Shinohara, 2010) |
| | | 2 ng/L | 1/4 | Japan | (Kameda et al., 2011) |
| WWTP sludge | | 0.54 – 17 µg/g dw | 7/8 | Sweden | (Brorström-Lundén et al., 2011) |
| | | 1.80 – 8.40 ng/g dw | 4/5 | China | (Zhang et al., 2011) |
| | | 1.53 – 133 ng/g dw<br>median 14 ng/g dw | 24/60 | China | (Ruan et al., 2012) |
| | | 120 – 200 ng/g dw | 5/5 | Japan | (Nakata and Shinohara, 2010) |
| storm water | | 0.13 – 0.17 ng/L | 3/4 | Sweden | (Brorström-Lundén et al., 2011) |
| refuse derived fuel (combustible municipal solid waste) | | 20 ng/g | 1/1 | Japan | (Watanabe and Noma, 2010) |
| landfill effluent | | 0.45 and 1.3 ng/L<br>particles:<br>4.3 µg/g dw | 2/3<br><br>1/1 | Sweden | (Brorström-Lundén et al., 2011) |
| pilot-scale waste incinerator | flue gas | 0.0042 µg/m³ | 1/1 | Japan | (Watanabe and Noma, 2010) |
| | fly ash | 0.049 ng/g | 1/1 | | |
| | bottom ash | 0.036 ng/g | 1/1 | | |
| foodstuff | seafood | max. ca. 1.4 ng/g ww | 6/7 | Japan | (Yanagimoto et al., 2011) |
| | imported meat | max. ca. 1.2 ng/g ww | 2/2 | | |
| | egg | ca. 0.6 ng/g ww | 1/1 | | |
| | vegetables, potatoes | max. ca. 0.3 ng/g ww | 5/8 | | |
| | cereals | ca. 0.5 ng/g ww | 1/2 | | |
| | soy | n.d. | 0/1 | | |
| | fruit | max. ca. 0.5 ng/g ww | 2/5 | | |
| | dairy products | n.d. | 0/4 | | |
| | clams | 1.0 – 8.5 ng/g ww (industrial pollution) ca. 2 ng/g ww (unpolluted) | 6/13<br><br>1/1 | USA | (Pruell et al., 1984). |

| | | | | |
|---|---|---|---|---|
| human adipose tissue | max. ca. 60 ng/g lw | 22/22 | Japan | (Yanagimoto et al., 2011) |
| | max. ca. 45 ng/g lw | 18/18 | South Korea | |
| | max. ca. 17 ng/g lw | 7/12 | Spain | |
| | max. ca. 11 ng/g lw | 12/12 | Poland | |
| | max. ca. 8 ng/g lw | 3/5 | India | |
| | max. ca. 5 ng/g lw | 10/24 | USA | |
| | n.d. | 0/? | China | |

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

Summary :

Studies on UV-327 are available from Sweden, Germany, Spain (and Portugal), USA, the Philippines, China and Japan (with certain data from other Asian countries and Poland).

The substance has been detected in air and air deposition, in dust from houses, roads and car cabins, in soil, surface water, sediments, aquatic organisms, water fowl, marine mammals, in WWTP influent, effluent and sludge, in storm water, landfill effluent, foodstuff, human adipose tissue, combustible municipal solid waste and in flue gas, fly ash and bottom ash of a pilot-scale waste incinerator.

In Swedish air concentrations up to several ng/m³ were detected. Samples from background sites may also contain UV-327 in measurable concentrations. In air deposition samples from Sweden a few hundred ng/m² were detected, with the highest concentration at a background site.

In road dust in Japan, house dust from private houses in Spain and the Philippines and in dust from a public building in Spain comparable concentrations were found (several to around one hundred ng/g). In house dust from the USA the concentration was higher (around 300 ng/g). In Swedish soil concentrations were up to a few µg/g dw, whereas in German soil the substance was not detected.

Measured concentrations in surface water may reach few ng/L (max. 6 ng/L) in Japan and were below 1 ng/l in Sweden, also at background sites. In suspended solids from German river water no UV-327 was detected. In sediments concentrations were usually around one to a few ng/g dw in China, the USA, European samples and Japan. At Japanese background sites concentrations around 1 ng/g dw were detected. In a polluted Japanese river with suspected point sources concentrations reached 190 ng/g dw. High concentrations of several µg/g dw were detected in Sweden, also at background sites. No explanation is offered for these high values.

Extreme concentrations up to the mg/g range were found downstream an American chemicals plant, at which UV-327 had been produced in the past. The maximum concentration in the sediment core was 0.2 mg/g seventeen years after production at the plant stopped. 25 years after production stop concentrations were still high in sediment cores (up to ca. 690 ng/g dw).

Concentrations in aquatic organisms varied. For Japanese marine organisms concentrations are given on a wet weight basis and usually range from below one up to a few ng/g ww. Similar values were found in the liver of Japanese water fowl. The blubber of marine mammals from Japan contained UV-327 at somewhat higher concentrations (max. 45 ng/g ww). Concentrations given on a lipid weight basis are higher, ranging from a few to a few hundred ng/g lw in marine organisms from Japan and the Philippines and mussels from the USA and 6 of 10 Asian countries. Highest concentrations (ca. 0.3 µg/g lw) were found in mussels from Korea and Hong Kong. Only UV-327 concentrations of Swedish fish are given on a dry weight basis. The highest value was measured in fish from a background site (ca. 10 µg/gdw). UV-327 is especially found in lipid of lower benthic

organisms collected from tidal flat areas. High concentrations were also found in fish from demersal habitat. UV-327 seems to be accumulated in the blubber of marine mammals.

In wastewater measured concentrations were few to several ng/L (max. 85 ng/L) in Spain and Portugal as well as in Japan. WWTP effluents often did not contain UV-327 in Spain and Japan. However, in individual samples from Japan, Spain and Portugal UV-327 was detected at concentrations of few to several ng/L (max. 31 ng/L in Portugal). In the Swedish study a lower detection limit was reached, showing UV-327 concentrations of ca. 0.1-0.5 ng/L in most WWTP effluents. A very high concentration of UV-327 was found in one sample of WWTP effluent particles investigated in Sweden (270 µg/g). UV-327 was usually found in WWTP sludge, but concentrations varied with lower concentrations in China (few to 133 ng/g dw), higher concentrations in Japan (max. 200 ng/g dw) and highest concentrations in Sweden (up to several µg/g dw). Some Swedish storm water samples contained UV-327 at low concentrations (around 0.1 ng/L).

Concentration of UV-327 in "refuse derived fuels" obtained from Japanese municipal solid waste after removing the incombustible materials was 20 ng/g (Watanabe and Noma, 2011). After treatment in a pilot-scale incinerator the concentration in the flue gas (final exit) was 0.0042 µg/m³, which is lower than concentrations measured in Swedish ambient air. Bottom ash contained 0.049 ng/g UV-327, fly ash 0.036 ng/g. In landfill effluents from Sweden low concentrations around 1 ng/L were detected, whereas a sample of particles from a landfill effluent contained UV-327 in high concentrations (4.3 µg/g dw).

Maximum concentrations of UV-327 in foodstuff analyzed in Japan were around 1 ng/g ww. In seafood collected from locations near industrial point sources in the USA concentrations were a bit higher (few ng/g ww). In human adipose tissue concentrations of few to several ng/g lw were found in Japan, South Korea, Spain, Poland, India and USA.

## 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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Dossier on 407-000-3: Information from dossier on EC 407-000-3 of former registration program according to Dangerous Substance Directive 67/548/EEC; confidential identity of the registrant

## 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**[8] | **UV-328** | **UV-327** | **UV-571** | **UV-928** | **UV-234** | **UV-360** |
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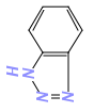
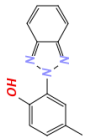
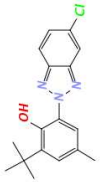
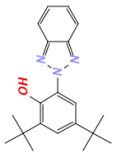
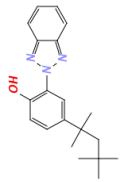
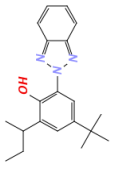
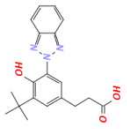
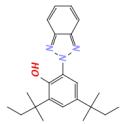
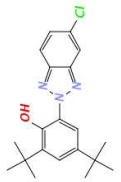
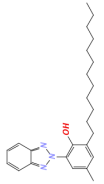
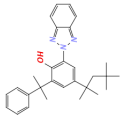
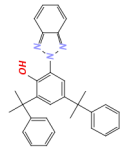
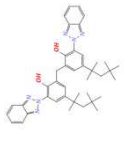
| |  |  |  |  |  |  |  |  |  |  |  |  |  |
| CAS No | 95-14-7 | 2440-22-4 | 3896-11-5 | 3846-71-7 | 3147-75-9 | 36437-37-3 | 84268-36-0 | 25973-55-1 | 3864-99-1 | 125304-04-3 | 73936-91-1 | 70321-86-7 | 103597-45-1 |
| EC No | 202-394-1 | 219-470-5 | 223-445-4 | 223-346-6 | 221-573-5 | 253-037-1 | - | 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 | 1.44[9] | 4.31[9] | | | | | | | | | | >6.5[10] | 4.2[11]; |

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

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

[10] 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**[8] | **UV-328** | **UV-327** | **UV-571** | **UV-928** | **UV-234** | **UV-360** |
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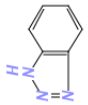
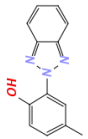
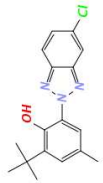
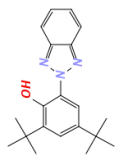
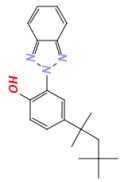
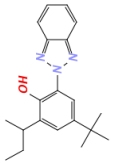
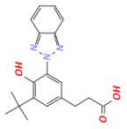
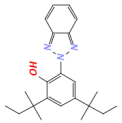
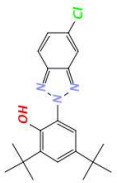
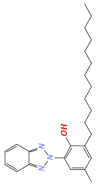
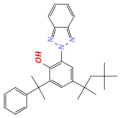
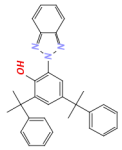
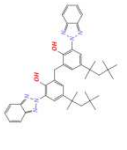
| |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Kow | | 4.2[10] | | | | | | | | | | | 12.7[11,12] |
| $pK_A$ | 8.37[13] | | | | | | | | | | | | |
| log Koc | | | | | | | | | | | | | 5.63[11] |
| Water sol. [mg/L] | 19800[14] | 0.173[15]; 0.8[16] | | | <1[10] | | | 0.015[16] | 0.022[16] | | | <0.04 (at 20°)[10] | <0.007[11] |
| Vapor pressure [Pa] | | | | | | | | | | | | | 6 $10^{-13}$ [11] |
| **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 |

[11] Data disseminated on ECHA-Homepage

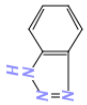
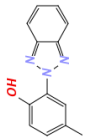
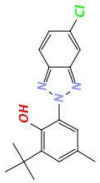
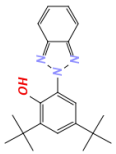
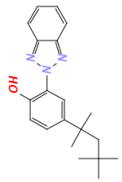
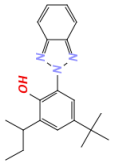
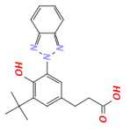
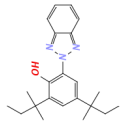
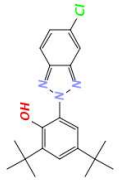
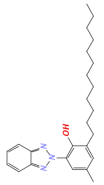
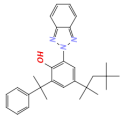
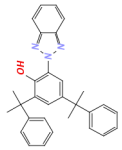
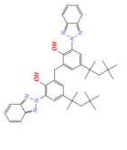
[12] This value is so large that is probably not reliable

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

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

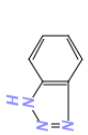
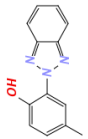
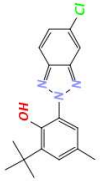
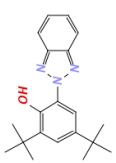
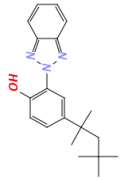
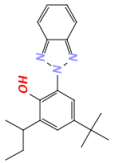
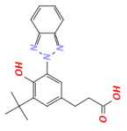
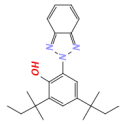
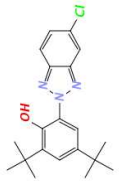
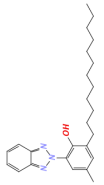
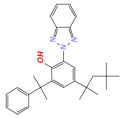
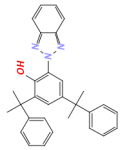
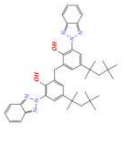
[15] US EPA Screening-LevelHazard Characterization Sponsored Chemicals Phenolic Benzotriazoles Category (2009)

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

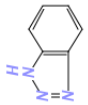
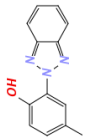
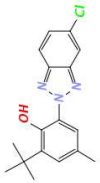
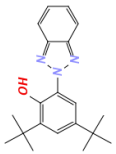
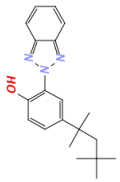
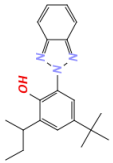
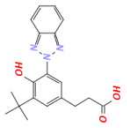
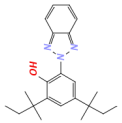
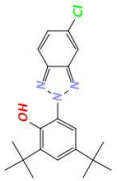
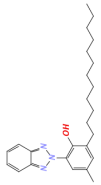
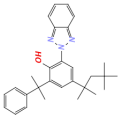
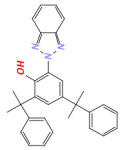
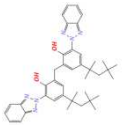
| **Acronym** | **1H-Benzotriazole** | **UV-P** | **UV-326** | **UV-320** | **UV-329** | **UV-350** | **M1**[8] | **UV-328** | **UV-327** | **UV-571** | **UV-928** | **UV-234** | **UV-360** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| |  |  |  |  |  |  |  |  |  |  |  |  |  |
| | BOD =2[17] | 0–2% after 28 days[15] | | BOD =0[17] | 0–1% after 28 days[15] | | | 2–8% after 28 days[15] | BOD =0[17] | | -4–3% after 28 days[18] | 3–8% after 28 days[15] | 5)[11]; Biodegradation in water <2% (84/499/CEE method 5)[11]; Biodegradation in water 0% (84/499/CEE method 5)[11] |
| Simulation tests | Primary degradation aerobic: $DT_{50}$=114 d anaerobic: | | | | | | OECD 308 aerobic: $DisT_{50}$ = 86 d (river system) $DisT_{11}$ = | | | | | | |

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

[18] 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**[8] | **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[17] | 1000 µg/L: 171-686; 100 µg/L: 181-410; 10 µg/L: 55-275[17] | 500 µg/L: 71-143; 50 µg/L: 258-1055; 5 µg/L: 721-1178[17] | 10 µg/L: 1945; **1 µg/L: 5905; 0.1 µg/L: 12041**[17] | | **1 µg/L: 20263; 0.1 µg/L: 34210**[17] | | 0.1 µg/L: 1121; 0.01 µg/L: 740-2148; **0.01 µg/L: 3681**[17] | 1 µg/L: 1203; **0.1 µg/L: 6283/8817; 0.01 µg/L: 7540**[17] | | | | |
| Field BAF calculat | | | | | | | | **0.012 µg/L: 6429**[19] | **0.012 µg/L: 5946**[19] | | | | |

[19] : 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**[8] | **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 20: Self Classification for UV-327 acc. to Regulation (EC) 1272/2008 (CLP)**

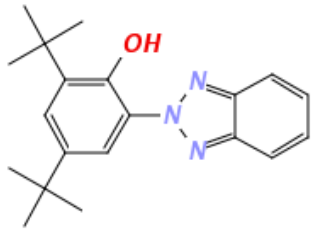
| Name / Tradename | EC-number | Hazard Class and Category Code(s) | Hazard Statement Code(s) |
|---|---|---|---|
| 2,4-di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol<br>UV-327 | 223-383-8 | Acute Tox. 4<br>Skin Irrit. 2<br>Eye Irrit. 2<br>STOT SE 3<br>STOT SE 2<br>STOT RE 2<br>Aquatic Acute 1<br>Aquatic Chronic 1<br>Aquatic Chronic 3<br>Aquatic Chronic 4 | H302<br>H315<br>H319<br>H335<br>H371<br>H373<br>H400*<br>H410<br>H412<br>H413 |

*The C&L inventory does contain the note that the Hazard Statement was derived by a study that did not consider all three trophic levels. Therefore the classification was derived by applying a safety factor of 100 on the available data and has an high uncertainty attached to it.

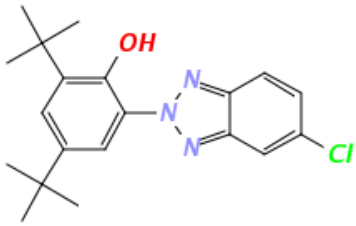
## ANNEX 3: ANALYSIS OF QSAR APPLICATION: PREDICTION OF LOG KOC FOR UV-320, -327, -328 AND -350

### A Information on substances and purpose

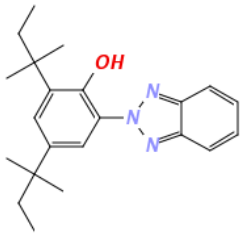
Molecule 1:

| | | |
|---|---|---|
| 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 | |

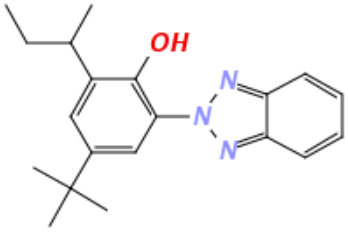
Molecule 2:

| | | |
|---|---|---|
| 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.[20]: 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" |

[20] w.a.: when applicable

| | | | |
|---|---|---|---|
| | | | Koc = (µg adsorbed/g organic carbon) / (µg/mL solution) [L/kg or mL/g] |
| **2 – Definition of Algorithm** | | | |
| Brief description of algorithm and/or link to full definition | Non-polar chemicals (i.e. compounds where no correction factor is needed):<br><br>$\log K_{oc} = 0.8679 \text{ Log } K_{ow} - 0.0004$<br><br>Polar chemicals (i.e. compounds where a correction factor is needed):<br><br>$\log K_{oc} = 0.55313 \text{ Log } K_{ow} + 0.9251 + \Sigma P_f N$ | 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:<br><br>within <= 0.20 - 44.2%<br><br>within <= 0.40 - 76.9%<br><br>within <= 0.60 - 93.0%<br><br>within <= 0.80 - 98.6%<br><br>within <= 1.00 - 100%<br><br>non-polar Training Set (n=68): $r^2$=0.877; std. dev.=0.478; avg. |

| | | | |
|---|---|---|---|
| | | | dev.= 0.371<br><br>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<br><br>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<br><br>Non-Polar Training Set: Online Help of KOCWIN, Appendix E<br><br>Polar Training Set: Online Help of KOCWIN, Appendix F | |
| Limits of the Applicability Domain | Molecular weight: 32.04-665.02 g/Mol<br><br>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.[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) | 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”<br><br>Koc = (µg adsorbed/g organic carbon) / (µg/mL |

[21] w.a.: when applicable

| | | | |
|---|---|---|---|
| | | | solution) [L/kg or mL/g] |
| **2 – Definition of Algorithm** | | | |
| Brief description of algorithm and/or link to full definition | log Koc = 0.5213 MCI + 0.60 + $\Sigma(P_f*N)$; MCI = $\Sigma(\delta i*\delta j)^{-0.5}$ | See Online Help of KOCWIN | MCI: Molecular Connectivity Index (in this case: First Order) mathematical approach to describe molecular topology<br><br>The equation was developed in a two step regression approach:<br><br>1. Derivation of equation without correction factors using a set of non polar chemicals<br>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:<br><br>within <= 0.20 - 44.2%<br><br>within <= 0.40 - 76.9%<br><br>within <= 0.60 - 93.0% |

| | | | |
|---|---|---|---|
| | | | within <= 0.80 - 98.6%<br><br>within <= 1.00 - 100%<br><br>non-polar Training Set (n=69): $r^2$=0.967; std. dev.=0.247; avg. dev.= 0.199<br><br>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<br><br>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<br><br>Non-Polar Training Set: Online Help of KOCWIN, Appendix E<br><br>Polar Training Set: Online Help of KOCWIN, Appendix F | |
| Limits of the Applicability | Molecular weight: 32.04-665.02 g/Mol | | |

| | | | |
|---|---|---|---|
| Domain | 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.[22]: 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 | Log $K_{OC} = 0.0168*M_0^X - 0.017*M_2^X - 0.040*M_3^X + 0.19*PM_{acc}^X - 0.27*M_{don}^X + 0.37$ 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 $-\sigma >$ | "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 molecules like partition coefficients |

[22] w.a.: when applicable

| | | | |
|---|---|---|---|
| | 1 e/nm$^2$ | "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). | 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 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 ($\Delta G_{hydr}$, log(vapor pressure), log $K_{octanol-water}$, log $K_{hexane-water}$, log $K_{benzene-water}$, log $K_{diethyl\ ether-water}$<br>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:<br><br>"Refinement and Parametrization of COSMO-RS", Andreas Klamt, Volker Jonas, Thorsten Bürger and John C. W. Lohrenz, *J. Phys. Chem.* | Original parameterization for COSMOtherm:<br><br>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 |

| | | | |
|---|---|---|---|
| | | *A* **102**, 5074-5085 (1998).<br><br>Log $K_{OC}$-formula:<br><br>"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). | |
| **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

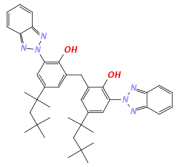
## QSAR Model: KOCWIN KOW-method, KOCWIN MCI-method and COSMOtherm ($K_{OC}$)

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 :<br>log $K_{OC}$ = 11.08<br>KOCWIN KOW-method :<br>log $K_{OC}$ = 8.22<br>COSMOtherm:<br>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

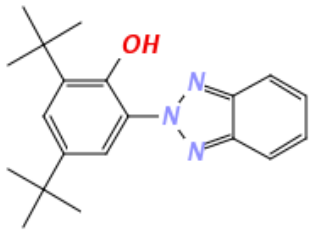
phenolic benzotriazoles were a experimental log $K_{OC}$ is reported, UV-360 was chosen as point of reference.

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

### A Information on substances and purpose

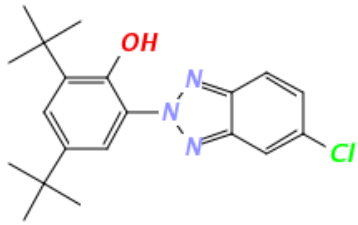
Molecule 1:

| | |
|---|---|
| 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 |

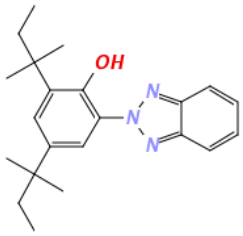



Molecule 2:

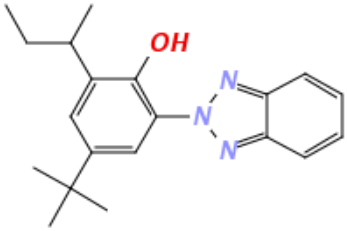
| | |
|---|---|
| Name: | 2,4-di-tert-butyl-6-(5-chlorobenzotriazol-2-yl)phenol (UV-327) |
| CAS Nr. | 3864-99-1 |
| EU Nr. | 223-383-8 |
| Smiles | c1(c(c(cc(c1)C(C)(C)C)C(C)(C)C)O)N(N=C2C=C3)N=C2C=C3Cl |



## 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.[23]: 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 | 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:<br>1. Derivation of $f_i$<br>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 | See Online help of KOWWIN, Appendix D | There are 157 different atoms and fragments defined and 278 correction factors that are employed when certain |

[23] w.a.: when applicable

| | | | |
|---|---|---|---|
| | leads to a correction instance occurs | | chemical classes or functional groups are present in the molecule for which an estimation is made |
| 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:<br>within <= 0.10 - 45.0%<br>within <= 0.20 - 72.5%<br>within <= 0.40 - 92.4%<br>within <= 0.50 - 96.4%<br>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 | Approximately 10.946 chemicals from | | |

| | | | |
|---|---|---|---|
| Type | 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:<br>within <= 0.20 - 39.6%<br>within <= 0.40 - 66.0%<br>within <= 0.50 - 75.6%<br>within <= 0.60 - 82.5%<br>within <= 0.80 - 91.6%<br>within <= 1.00 - 95.6%<br>within <= 1.20 - 97.7%<br>within <= 1.50 - 99.1% | | Details available in Online help of KOWWIN |
| **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.[24]: 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)= $\int p^i(\sigma)(\mu_{water}(\sigma;T) - \mu_{octanol}(\sigma;T))d\sigma + \mu_i^C(water, T) - \mu_i^C(octanol,; T)$, 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 $\underline{r} = \Sigma_i x_i^* r_i$ | "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 |

[24] w.a.: when applicable

| | | | |
|---|---|---|---|
| | and $q = \Sigma_i x_i * q_i$ | | Mechanical methods. Due to a treatment with statistical thermodynamics the macroscopic properties of interacting 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; $\lambda_0$, $\lambda_1$, $\lambda_2$: 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 | Original parameterisation: 225 small- and medium-sized organic compounds with H, C, O, N, Cl atoms. The fitting was done for 650 | | While the principle theory is applicable for all elements, the practical implementation needs some specific parameters to the |

| | | | |
|---|---|---|---|
| description of it | experimental room-temperature parameters ($\Delta G_{hydr}$, log(vapor pressure), log $K_{octanol\text{-}water}$, log $K_{hexane\text{-}water}$, log $K_{benzene\text{-}water}$, log $K_{diethyl\ ether\text{-}water}$ | | 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

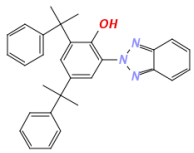
## QSAR Model: KOWWIN and COSMOtherm ($K_{OW}$)

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 :<br>log $K_{OW}$ = 7.67<br>COSMOtherm:<br>log $K_{OW}$ = 8.30 |
| **Predicted endpoint** | See above |
| **Experimental endpoint** | > 6.5 |
| **Statistical performance** | - |

Rationale for the selection of similar substances

Substanc 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 STUDY RESULTS FOR UV-320, UV-327, UV-328, UV- 350

### 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 21: 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 22: Concentrations of phenolic benzotriazoles in air and atmospheric deposition in Sweden**

| Substance | Air | | Deposition | |
|---|---|---|---|---|
| | detected in x of y samples [x/y] | concentration [ng/m³] | detected in x of y samples [x/y] | deposition flux [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 23: 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 24: 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 25: 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 26: Concentrations of phenolic benzotriazoles in effluent landfill and storm water in Sweden**

| **Substance** | **effluent landfill** | | **storm water** | |
|---|---|---|---|---|
| | detected in x of y | concentration [ng/L] | detected in x of y | concentration [ng/L] |

| | samples [x/y] | | samples [x/y] | |
|---|---|---|---|---|
| **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 27: 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 28: 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 29: 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 30: 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 31.

**Table 31: 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 32: 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<br>3.4 | < 0.15 |

**Table 33: 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 34: 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 35: 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 36: 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 37: 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 (M1-M12)** | Occurrence | 5/12 | 6/12 | 8/12 |
| | 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 38: 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 39: 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 40: 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 41: 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 42: 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 43: 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<br>two extreme values: 2930 and 3390 | 67.8 |
| **UV-327** | 24/60 | 1.53 – 133 | 14 |
| **UV-328** | 58/60 | 3.54 – 213<br>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 44: 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 45: 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

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## 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 |

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| 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 |

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|---|---|
| $r^2$ | 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 |