
Comments from a downstream user of UV-328 (EC 247-384-8). Public Consultation Candidate List

Document containing a downstream user's comments to the Annex XV dossier on UV-328. This document includes non-confidential information only.

Purpose: Input to stakeholders

Date:

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**Submitted by a Downstream User
(confidential)**

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1. Introduction

This document describes the non-confidential comments of a downstream user regarding the Annex XV dossier “*Proposal for identification of a substance of very high concern on the basis of the criteria set out in REACH article 57*” for the substance 2-(2H-benzotriazol-2-yl)-4,6-ditertpentylphenol (UV-328) with EC number 247-384-8” prepared by the German Member State Competent Authority (MSCA-DE).

The submitter of these comments is a downstream user of the substance 2-(2H-benzotriazol-2-yl)-4,6-ditertpentylphenol (UV-328) with EC number 247-384-8 (UV-328).

The information on use and use conditions (confidential) is important in view of conclusions on the (non) exposure potential. The other comments (non-confidential) are important in light of the hazard assessment and in light of the selection of the most appropriate risk management route.

Our comments describe the following topics:

- 1. Incomplete assessment of available data:** The downstream user considers the annex XV document to be rather a plea for classifying the substance as a PBT / vPvB and not a balanced assessment of the PBT status of the substance. The lack of transparency and the selective use of data and of guidances led to this conclusion.
- 2. Risk management route: Authorisation is not the appropriate route**
 - a. An important concern is mentioned with regard to manufacturing sites and import of articles containing UV-328. This cannot be managed by authorisation, only by restriction of the uses which lead to a non-acceptable risk.
 - b. We have implemented measures to enable minimisation of emissions. Under a socio-economic analysis for restriction it would become clear that this use is not to be restricted.
 - c. For several uses of UV-328 there may be alternatives available, but not for our downstream use.

2. Comments

2.1. Incomplete assessment of available data

The Annex XV dossier is an extensive document with the goal to prove the PBT and/or vPvB properties of UV-328. However, important information with regard to the hazard data is missing. It is therefore not possible for a third party to evaluate in full the assessment made by the German Member State Competent Authority (MSCA-DE). For instance, only interpreted results (to prove PBT status) from study reports are presented, but not the raw data. The reader does not have access to these data. As a result, scrutiny of the assessment is not possible. Hence, the lack of transparency infringes the right of industry to comment.

In the Annex XV dossier it is stipulated that the conclusion is based on a Weight of Evidence approach. However, data indicating that UV-328 is not persistent and/or not bio-accumulative are not used in the Weight of Evidence, although such data are available. The Annex XV dossier does not provide a scientific justification why these data have not been considered in the Weight of Evidence. As mentioned, the Annex XV dossier aims to prove that UV 328 is PBT and/or vPvB. This is done by selecting those data that prove the cause, while neglecting those that prove the opposite.

2.1.1. Water sediment simulation tests

2.1.1.1. Read across justification

The Weight of Evidence (WoE) with regard to persistence is almost entirely based on read-across to the substance M1, a degradation product of EC 407-000-3. The read-across is justified only on basis of apparent similarity of chemical structure: “*Based on this structural relationship they should have similar physico-chemical properties*” (page 19 of the Annex XV dossier). However it is not clear (not transparent) how the MSCA came to this conclusion. It is e.g. not discussed how the carboxylic acid group influences the environmental behavior of M1 compared to the tert-amyl group of UV-328.

Also, no further evidence is provided of similar behavior which is to be expected on the basis of the similar structure. Indeed, a read-across justification should be accompanied by a comparison of physico-chemical and other properties of (i) the substance under assessment and of (ii) the read-across substance to demonstrate the validity of the read-across (ECHA Guidance on Information Requirements and Chemical Safety Assessment R6: QSARs and grouping of chemicals; Section R.6.2.3.1). It is argued by MSCA-DE that no experimental data is available to proof the structural similarity. However, the properties estimated on the basis of the structure of the substances by means of EPIWeb 4.1 QSAR, indicate significant differences in physico-chemical properties for UV-320, UV-328, M1 and UV-327. It seems that the structural similarity of the different substances is selectively used to proof the PBT properties. QSAR estimations are provided in Table 1 for the properties as presented as unknown in Table 6 of the Annex XV dossier.

Table 1: Physico-chemical properties of UV-320, UV-328, M1 and UV-327

	UV-320	UV-328	M1	UV-327
Mol. Weight [g/mol]	323.4	351.5	339.4	357.9
Log Kow	6.27 ^c	> 6.5 ^a	3.01 ^c	6.91 ^c
Water Solubility [mg/L]	0.15 ^c	0.015 ^b < 0.001 (20°C) ^a	218 ^c	0.022
Vapor Pressure [Pa]	5.71E-08 ^c	0.000005 (20°C) ^a	6.98E-10 ^c	1.37E-08 ^c

a) According to the registration dossier

b) According to Lopez-Avila, Hites (1980)

c) According to EPIWeb 4.1

From this comparison of physicochemical data it is clear that M1 differs significantly from the other 3 substances. M1 has a water solubility that is more than a factor 1000 higher and a log Kow value that is 3 units lower. These observations can be attributed to the presence of the carboxyl group in the chemical structure of M1. The above described physicochemical properties have an important impact on the environmental behavior of the concerned substances, e.g. by influencing the distribution over the different compartments and the tendency to adsorb to solid matter. As a consequence, it can be concluded that the use of the read-across substance M1 for the purpose of the persistency assessment is not scientifically justified and not (sufficiently) substantiated.

In the Annex XV dossier the MSCA-DE acknowledges that they have no evidence on basis of physico-chemical properties, neither on analytics of breakdown products. We therefore conclude that the read-across does not comply to the ECHA requirements. As the read-across justification itself is poor, the entire WoE assessment on persistence is highly questionable.

2.1.1.2. OECD 308 test

For persistence reference is made to a test on EC 407-000-3 performed according to the OECD 308 method. It is stipulated that NERs (non-extractable residues) are being formed. The term NERs has been used in several fora under different definitions, e.g. ECETOC workshop 2012 (Paris) where UBA presented on 3 types of NERs. From the Annex XV dossier on UV-328, we have the following questions with regard to interpretation of the data:

- What is meant exactly in this case by the term NERs as a clear definition is not given?
- How has the chemical analysis of the NERs been performed? ;
- How was the chemical analysis performed on M1 to qualitatively and quantitatively define M1 to be adsorbed to sediment? Which extraction methods have been used? This is important information to differentiate between adsorption and NER formation. Under severe extraction conditions, a covalent bond can be broken, leading to a false conclusion that it concerns adsorption instead of NER formation. As NERs are no longer bio-available due to their chemical or strong physical bond to soil and/or sediment, they are to be considered as a removal pathway (ECHA guidance R7B¹).
- Has the MSCA assessed NERs as a removal pathway, as is stipulated in the ECHA guidance R7B?

ECHA guidance R7B: Knowledge of **bound residues and incorporation into biomass** also needs to be considered and should be seen as a **potential removal pathway**. The OECD 308 (2002) Guideline advises as follows: “Bound residues represent compounds in soil, plant or animal that persists in the matrix in the form of

¹ http://echa.europa.eu/documents/10162/13632/information_requirements_r7b_en.pdf

*the parent substance or its metabolite(s) after extractions. The extraction method must not substantially change the compounds themselves or the structure of the matrix... In general, **the formation of bound residues reduces the bioaccessibility and the bioavailability significantly** (1) [modified from IUPAC 1984 (2)]."*

Extraction of the sample, often with a suitable organic solvent is generally repeated 3 or 4 times until no further yield is achieved. Typically a range of solvents are used of increasing polarity (e.g. methanol, acetone, acetonitrile and hexane etc.) under ambient conditions. If the entire residual radioactivity cannot be recovered then appropriate solvent may be mixed with weak acids or bases or coupled to ultrasonic extraction. This aims to provide different conditions that may lead to the chemical or metabolite being released back into solution. Finally, the use of strong acids, bases or refluxing could undoubtedly extract the sample more thoroughly but could alter both the compounds of interest and the matrices. Such severe extraction techniques are rarely if employed in e.g. routine soil or sediment/water testing. The extraction methods and efficiencies as well as analytical methods and detection limits should always be reported.

These considerations should aid in determining the following environmental assessments for classification, PBT/vPvB and potential exposure.

- Not only the ECHA guidance refers to bound residues as a removal pathway. Also the Guidance on Estimating Persistence and Degradation Kinetics (FOCUS, 2006), defines degradation as the chemical transformation into another compound, either by break down or by chemical transformation into larger molecules. The transformation of a substance into NERs is thus contributing in the degradation half-life (DegT50).

*Focus 2006: Generic guidance for Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration² (JRC-Europe): **Degradation products***

*All substances resulting from biotic or abiotic transformation reactions of the test substance including CO₂, microbial biosynthetates, and **products that are in bound residues.***

Guidance for Evaluating and Calculating Degradation Kinetics in Environmental Media (US-EPA)³

Degradation** (also transformation): Degradation or transformation processes transform **one compound to another through chemical or biological reactions in different environmental compartments.** Degradation usually breaks down substances by such processes as hydrolysis or photolysis, but **may also result in larger molecules by such processes as biosynthesis or polymerization.

Although the MSCA-DE refers to FOCUS and the correlated guidance, it is unclear whether the kinetics of NERs formation is used as a contributing factor in DT50 (disappearance half-life) and in DegT50. Only then the assessment complies to the ECHA guidance that NERs shall be considered a removal pathway.

On basis of the results of the OECD 308 (p33, Table 10 of the Annex XV dossier) one can see that M1 is not persistent in sediment for the river system, whereas for the pond system the DT50 exceeds the trigger criteria of Annex XIII. The results are conflicting, however MSCA-DE draws the conclusion of very persistent on basis of the highest DT 50 values in the test results. This conclusion again demonstrates the selective use of data to unilaterally proof the PBT status.

It would be scientifically more interesting to question and investigate the reason for the diverging test results. What does this say about the precision and/or accuracy of the test?

² http://focus.jrc.ec.europa.eu/dk/docs/FOCUSkineticvc_1_0_Nov23.pdf

³ <http://www.epa.gov/oppfead1/international/naftatwg/guidance/degradation-kin.pdf>

The reliability of OECD 308 is under scientific discussion (e.g. ECETOC Workshop, 2012, Paris). As a result a research program has been started within the CEFIC LRI programme, with regard to the interpretability of OECD 308 and OECD 309 in the context of PBT assessments under REACH⁴. The research program is ongoing and after contacting Mrs. Kathrin Fenner, the lead of the project, we understood that results are not expected before 2015. However, in this case of UV-328 MSCA-DE draws the conclusion that UV-328 is very persistent, even when the test results are conflicting and when the interpretability of the test used is under scientific investigation.

One could even argue that the higher DT50 value for pond systems compared to river systems (Table 10, page 33) are not representing longer degradation times, but are an indication of NER formation. Indeed, at higher organic carbon content, there is increased chemical bonding, resulting in increased NER formation. Hence, the DT50s should account for NER formation in the calculation, potentially resulting in a different conclusion on persistence.

2.1.2. Biodegradation in Soil

For persistency in soil the Annex XV dossier refers to Lai et al., 2014 with regard to a simulation field study (p29). The study considers Benzotriazole and Tolyltriazole as well as several phenolic benzotriazoles (UV-326, UV-327, UV-328, UV-329 and UV-P).

The test derives two DT50 values from

- Test T1 with a single application of sludge on agricultural land
- Test T2 with multiple applications (4) of sludge on agricultural land

The concentrations of the substances in soil are measured in an extract from the soil. The extract is obtained using 50/50 v/v methanol/dichloromethane as a solvent and this at 120°C for 5 minutes in two cycles. This can be considered as a severe extraction method, extracting species which can be considered as NER (ECETOC TR No. 117).

The results of the measurements (for UV-328) are shown in Figures 13 and 14 in Annex XV (p31). Both graphs depict a plateau at the right hand side. The level of the plateau is for T2 about four times as high as for T1. Based on this observation it could be concluded that the level of 3 ng/g, which is about constant for the 5 last months in T1, are bound residues that are biologically non-available. This concentration is expected to accumulate over multiple applications, as is the case for T2. Indeed, in T2 there are 4 applications of sludge and the level of bound residues is also about 4 times higher (12-15 ng/g) than in test T1 (3 ng/g), where a single application was used. The presence of a relative high level of NER in the system affects the calculation of the DegT₅₀ significantly. For T1 in 2011 this means that all bio-available substance has disappeared from the system within 3 months. With a linear rate this would result in a DegT₅₀ of 45 days, much lower than the calculated DT₅₀. The reason is that the DT₅₀ calculated in the Annex XV dossier assumes that all extracted product is bio-available, which it is not.

In general, the interpretation of the tests does not take sufficiently into account the fact

- That NERs are formed
- That the concentration measured with the severe extraction method also contains the NERs which are non-bio available
- Non-bio available NERs, as a removal pathway, contribute to the DT₅₀ and the DegT₅₀

In the conclusion of that section in the Annex XV dossier, it is stated that the DT₅₀ values are to be considered as “*best case assessment*” a.o. because NERs were not considered. However as demonstrated above, in the simulation field study by Lai et al., 2014, NERs were implicitly

⁴ Kathrin Fenner et al: Persistence testing at the sediment-water interface: Too much effort for too little data?, <http://www.cefic-lri.org/uploads/Posters%20LRI%20workshops%202009-2013/ECO18%20Persistence%20testing%20at%20the%20sediment-water%20interface.pdf>

included in the derivation of the results due to the choice of severe extraction method (ECETOC TR. 117), but they were not considered for the interpretation of the results. It seems that the interpretation by MSCA-DE includes the NERs fraction into the calculation of DT_{50} and $DegT_{50}$, whereas this should be done on the available fraction only. In that case the DT_{50} and $DegT_{50}$ would be significantly lower. The impact of NERs on the calculation of DT_{50} and/or $DegT_{50}$ is depicted in Figure 1.

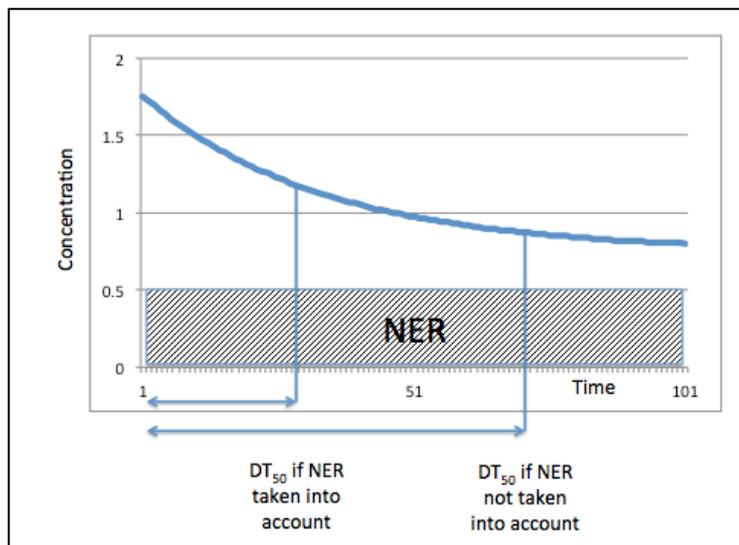


Figure 1: Impact of NERs on calculation of DT_{50} and $DegT_{50}$

2.1.3. Field data

In section 3.1.3 (p34) there is confusing information regarding the presence of UV-327/328 upstream of the production plant. On the one hand it is stated that in the sludge of the WWTP the substances were found, but this WWTP is mentioned to be upstream of the former chemical plant: “*There was and still is a municipal wastewater treatment plant situated a certain distance upstream of the (former) chemical plant*”. On the other hand it is clearly stated that UV-327/8 were not found in sediment upstream of the chemical plant.

For persistence reference is made to these field data (Section 3.1.3, p34). Also for these test results it is not clear how the analysis of the sediment cores is made. Which extraction methods have been used? As mentioned above with regard the OECD 308 test, information on analytical techniques used is paramount to define the distinction between adsorption and NER formation. Adsorption is understood to be reversible; hence the substance can become bio-available again in the future. NERs on the other hand are understood to be non-reversible and thus no longer bio-available, i.e. a safe sink. In the latter case, the substance is considered to be not persistent (ECHA guidance R7B). From the field test data presented in the Annex XV dossier, we conclude that it most probably concerns NERs that are no longer bio-available. In that case it concerns a safe sink.

The field tests show the presence of UV-328 in the environment. From the Annex XV dossier it cannot be distinguished whether UV-328 is simply adsorbed or irreversibly bound to the soil. In the latter case, UV-328 has to be considered as a NER and would not be bio-available. Hence, it is not leading to persistence according to the ECHA guidance R7B. The Annex XV dossier provides no transparency on this matter. Even more, MSCA-DE does not seem to consider this possibility as this is nowhere discussed in this section.

2.1.4. Bioaccumulation

For bioaccumulation reference is made to a publication of Nakata et al. The former Annex XV dossier (2013) also made reference to this publication. More specifically, MSCA-DE referenced a BAF value of 36.000 for UV-328. We have demonstrated in our comments of 2013 that this was a serious mistake in the Annex XV dossier and moreover that from this study a conclusion on bioaccumulation could not be drawn. We regret to see that in the Annex XV dossier of 2014, the publication is again used as evidence of the bioaccumulative potential of UV-328. This time MSCA-DE does not refer anymore to the BAF as a value reported in the publication, which indeed it is not, but a BAF is still mentioned. For the reader it is not clear that this is a calculation made by MSCA-DE and not by the author. This in itself is already misleading, but more importantly, on basis of the publication itself we cannot re-construct the MSCA's value of 33.300 for BAF. We are of the opinion that the calculation by MSCA-DE is erroneous and shall therefore be disregarded in the weigh of evidence.

Reference is also made to two BCF studies. One study dates from 2007, the other one from 2000. For the first BCF study (2007) a table is provided with BCF values per tissue. The data of the overall BCF is not provided in the Annex XV report. In the registration dossier an overview table of the overall BCF per fish is provided, after 12, 2, 40, 50, 60 days of exposure at two different concentrations. The BCF values are all below 2000, varying between 870 as a minimum and 1700 as a maximum. This would indicate that UV-328 is not bioaccumulative.

For the second BCF study (2000) an overview table is given for the overall BCF values per fish after 2, 4, 6 and 8 days of exposure at two different concentrations. The BCF values range from 1270 to 5580. This could indicate that UV-328 is bio-accumulative.

Only those test results are presented in the Annex XV dossier that fits the purpose of determining UV-328 as a PBT and vPvB, even though both studies are equally Klimisch rated as a K2. This is scientifically incorrect use of information.

It would be scientifically correct to investigate the reason for the diverging test results on bioaccumulation, instead of drawing a conclusion on part of the data only. UV-328 is a lipophilic substance with a high tendency to adsorb to solid matter. In the OECD 305 guideline⁵ it is noted that for strongly hydrophobic substances a dietary test (BMF) is recommended, due to the constraint of achieving a stable aqueous concentration. Hence, for UV-328 the BCF study could lead to incorrect conclusions, whereas a BMF study is more applicable. Indeed, the aquatic BCF studies were performed in a flow-through system. The continuous addition of UV-328 stock solution to the test tanks was intended to keep the concentration of UV-328 constant in the water. However, due to UV-328's high Koc values reflecting a tendency to adsorb to glass surfaces of the test chambers as well as to organic material, a portion of the added UV-328 will likely adhere to the fish feed added to the tanks. As a consequence, the fish will be exposed to UV-328 via the aquatic and additionally through the dietary route. Since the calculation of the BCF value only accounts for the aquatic concentration of the test chemical, the calculated BCF values will result in over-estimations.

⁵ OECD 305 guideline: <http://www.oecd.org/chemicalsafety/testing/49190738.pdf>

2.2. Risk Management Route

2.2.1. Authorisation versus Restriction

(1) Manufacturing of UV-328 and Import of finished goods containing UV-328

The Annex XV dossier describes significant exposure as a result of the manufacturing of UV-328. MSCA-DE demonstrates this in several monitoring studies near manufacturing plants world-wide (Annex XV dossier, p 34, 40, 55, 62, 151), where UV-328 is found in several environmental compartments even many years after shut-down of the production.

The Annex XV dossier also raises the concern on the import of finished goods containing UV-328 or similar UV-stabilisers (p 131 of Annex XV dossier, reference to Brorström-Lundén et al, 2011). For articles, this then results in a wide dispersive use and/or potential exposure of consumers. **The proposed hazard properties of PBT/ vPvB (non-threshold) combined with the exposure information** as provided in the Annex XV dossier results in a **conclusion of risk to human health or the environment that is not adequately controlled**.

Neither manufacturing of UV-328, nor the import of articles which pose a risk to human health or the environment that is not adequately controlled, is regulated by means of Authorisation and can only be regulated by means of Restriction. It should therefore be considered to restrict the conditions of manufacturing of UV-328 and the import of those articles that lead to risk.

(2) EU-wide risk, not adequately controlled

In the Annex XV dossier for UV-328 reference is made to monitoring data (Annex XV dossier, p 34, 40, 47, 55, 57, 58, 62, 145, 151), by which MSCA-DE demonstrates the presence of UV-328 in several environmental compartments, in seafood, in meat and in human adipose tissues. The concentrations measured raise concern for the MSCA with regard to the safety of human health and environment.

On basis of the inherent properties of UV-328 as deducted by the MSCA in the Annex XV dossier and on basis of the measured data (monitoring) described in several studies world-wide, for several compartments (see also Annex XV dossier), it could be concluded that, if there is a risk, it concerns a EU-wide risk related to certain uses of UV-328 and moreover that this risk is not adequately controlled. The Annex XV dossier relates this risk to the manufacturing sites of the UV-stabilisers, as well as to the related certain consumer uses, such as the use of UV-stabilisers in coatings and in cosmetics, e.g. sun protection agents.

With reference to Title VIII (Restrictions), Articles 68.1, 69.1 and 69.4 of REACH, **the more appropriate risk management route is Restriction and not Authorisation**. Art. 69.1: *“If the Commission considers that the manufacture, placing on the market or use of a substance on its own, in a mixture or in an article poses a risk to human health or the environment that is not adequately controlled and needs to be addressed, it shall ask the Agency to prepare a dossier which conforms to the requirements of Annex XV (restriction).”*

2.2.2. The use of UV-328

Detailed information on the use contains Confidential Business Information. This information is submitted to ECHA and the Member State Competent Authorities confidentially.

In summary, the use of UV-328 by the submitter of the comments, a downstream user, does not constitute a wide dispersive use (limited number of sites, limited or no release). Even more, downstream there is very limited or no exposure.

2.2.3. Information on alternatives

Detailed information on alternatives contains Confidential Business Information. This information is submitted to ECHA and the Member State Competent Authorities confidentially.

For several uses of UV-328 there may be alternatives available, but not for the use at this downstream user.

2.2.4. Prioritisation ranking

This paragraph is only of importance in case the regulator would decide to manage the potential risk by means of authorisation, which we believe would not be the appropriate risk management route.

In February 2014, ECHA released the following publication: "*Prioritisation of substances of very high concern (SVHCs) for inclusion in the Authorisation List (Annex XIV)*".

With regard to wide dispersive use, a conclusion is drawn on basis of:
Industrial use, professional use or consumer use.

We emphasize that the uses where there is a potential risk for exposure, although very small, are industrial uses.

It needs to be noted that in the registration dossiers, there is also an article category defined, because UV-328 can be included in the final article. However, in the article UV-328 is fully enclosed and does not result in any exposure. It would therefore be a significant overestimate to give UV-328 a ranking of 15 for wide dispersive use. Only the ranking for industrial use is relevant in this case.

2.3. Final Conclusions

We conclude that the Annex XV dossier as presented by MSCA-DE

- 1. Is a plea for classifying UV-328 as a PBT / vPvB on the basis of an incomplete assessment of available data.** The Annex XV dossier does not constitute a balanced assessment of the PBT status of the substance. The lack of transparency and the selective use of data and of guidances by the MSCA-DE is demonstrated in this document. More specifically, we question whether the MSCA-DE's conclusion on persistence accounts for the formation of NERs. It is clear that NERs are being formed, which according to the ECHA guidance R7B shall be considered as a removal pathway (not bio-available, not bio-accessible).
- 2. Risk management route: Authorisation is not the appropriate route**
 - a. An important concern is mentioned with regard to manufacturing sites and import of articles containing UV-328. This cannot be managed by authorisation, only by restriction of the uses which lead to a non-acceptable risk.

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- b. As downstream user we have implemented measures to enable minimisation of emissions. Under a socio-economic analysis for restriction it would become clear that this use is not to be restricted.
 - c. For several uses of UV-328 there may be alternatives available, but not for the use at this downstream user.