Committee for Risk Assessment

RAC

Opinion

proposing harmonised classification and labelling
at EU level of

decanoic acid

EC number: 206-376-4
CAS number: 334-48-5

CLH-O-0000002590-79-03/F

Adopted

6 June 2013

6 June 2013

CLH-O-0000002590-79-03/F

OPINION OF THE COMMITTEE FOR RISK ASSESSMENT ON A DOSSIER PROPOSING HARMONISED CLASSIFICATION AND LABELLING AT EU LEVEL

In accordance with Article 37 (4) of (EC) No 1272/2008, the Classification, Labelling and Packaging (CLP) Regulation, the Committee for Risk Assessment (RAC) has adopted an opinion on the proposal for harmonised classification and labelling (CLH) of:

Chemicals name: decanoic acid

EC number: 206-376-4

CAS number: 334-48-5

The proposal was submitted by **Austria** and received by the RAC on **21 June 2012.**

In this opinion, all classifications are given firstly in the form of CLP hazard classes and/or categories, the majority of which are consistent with the Globally Harmonised System (GHS) and secondly, according to the notation of 67/548/EEC, the Dangerous Substances Directive (DSD).

PROCESS FOR ADOPTION OF THE OPINION

Austria has submitted a CLH dossier containing a proposal together with the justification and background information documented in a CLH report. The CLH report was made publicly available in accordance with the requirements of the CLP Regulation at ***http://echa.europa.eu/harmonised-classification-and-labelling-consultation*** on **21 June 2012**. Concerned parties and Member State Competent Authorities (MSCA) were invited to submit comments and contributions by **6 August 2012**.

ADOPTION OF THE OPINION OF THE RAC

Rapporteur, appointed by RAC: **Helmut Greim**

Co-rapporteur, appointed by RAC: **José Luis Tadeo**

The opinion takes into account the comments provided by MSCAs and concerned parties in accordance with Article 37(4) of the CLP Regulation.

The RAC opinion on the proposed harmonised classification and labelling was reached on **6 June 2013** and the comments received are compiled in Annex 2.

The RAC Opinion was adopted by **consensus**.

OPINION OF THE RAC

The RAC adopted the opinion that **decanoic acid** should be classified and labelled as follows:

Classification and labelling in accordance with the CLP Regulation

	Index No	International Chemical Identification	EC No	CAS No	Classification		Labelling		
					Hazard Class and Category Code(s)	Hazard statement Code(s)	Pictogram, Signal Word Code(s)	Hazard state-ment Code(s)	Suppl. Hazard statement Code(s)
Current Annex VI entry									
Dossier submitters proposal		decanoic acid	206-376-4	334-48-5	Skin Irrit. 2 Eye Dam. 1 Aquatic Chronic 3	H315 H318 H412	GHS05 Dgr	H315 H318 H412	
RAC opinion		decanoic acid	206-376-4	334-48-5	Skin Irrit. 2 Eye Irrit. 2 Aquatic Chronic 3	H315 H319 H412	GHS07 Wng	H315 H319 H412	
Resulting Annex VI entry if agreed by COM	607-709-00-X	decanoic acid	206-376-4	334-48-5	Skin Irrit. 2 Eye Irrit. 2 Aquatic Chronic 3	H315 H319 H412	GHS07 Wng	H315 H319 H412	

Classification and labelling in accordance with DSD:

	Index No	International Chemical Identification	EC No	CAS No	Classification	Labelling	Concentration Limits
Current Annex VI entry							
Dossier submitters proposal		decanoic acid	206-376-4	334-48-5	Xi; R38-41 N; R51/53	Xi; N R: 38-41-51/53 S: (2-)26-36/37/39-45-46-61	
RAC opinion		decanoic acid	206-376-4	334-48-5	Xi; R36/38 N; R51-53	Xi; N R: 36/38-51/53 S: (2-)46-61	
Resulting Annex VI entry if agreed by COM	607-709-00-X	decanoic acid	206-376-4	334-48-5	Xi; R36/38 N; R51-53	Xi; N R: 36/38-51/53 S: (2-)46-61	

SCIENTIFIC GROUNDS FOR THE OPINION

RAC general comment

The only hazard classes considered by RAC were those of skin irritation/corrosion, eye irritation, respiratory irritation and the environment.

Please note that references cited here can be found in the CLH report and/or the background document to the opinion; references not quoted in the above documents are however included at the end of this opinion for the sake of convenience.

HUMAN HEALTH HAZARD ASSESSMENT

RAC evaluation of skin irritation/corrosion

Summary of the Dossier submitter's proposal

No specific guideline studies on irritation or corrosion with decanoic acid are reported in the CLH report. The dossier submitter therefore presented a weight of evidence approach and used this to derive a classification. Evidence from human volunteer tests, QSAR analysis and from the structurally similar nonanoic and octanoic acid were considered.

Several human volunteer patch test studies conducted with Octanoic, Nonanoic and Decanoic acid are described in the CLH report (Jirova et al., 2008; Robinson et al., 1999; Wahlberg, 1983 and Andersen et al., 1995). These all indicated that the substances were at least irritating to skin but most studies terminated exposure when volunteers showed signs of irritation. A transcutaneous electrical resistance test (TERT, York et al., 1996) indicated that decanoic acid was non-corrosive (29.9 kΩ/disc) while Jirova et al. (2008), using the EpiDerm in vitro skin irritation test, concluded that nonanoic and decanoic acid were at least irritant to skin. The ToxTree QSAR developed by the European Chemicals Bureau (ECB) tool indicated that octanoic, nonanoic and decanoic acids were borderline irritating or corrosive to the skin.

One non-GLP compliant, skin irritation study in rabbits using 100% decanoic acid was reported in the CLH report (Smyth et al., 1962), indicating severe skin irritation (reporting a score of 5 out of 10), but the study did not use standard test scoring and the report included no information on reversibility. An acute dermal toxicity test in rats using 25% Decanoic acid in polyethylene glycol indicated irritation to skin (erythema grade 1-2, reversible after 14 days, Talvioja, 2006). Application of 70% decanoic acid in acetone:olive oil in a mouse local lymph node assay three times over three consecutive days resulted in slight irritation while 50% and 25% application revealed no irritation (Weber, 2006). The dossier submitter includes three studies using nonanoic acid as supportive information, all showing severe irritation of nonanoic acid at or above 22% concentration (Otterdijk, 2001b, c and d).

The dossier submitter concluded that decanoic acid is at least irritating to the skin but based on the TERT study (York, 1996) argues that it should not be considered corrosive and therefore proposes a classification as Skin Irrit. 2 – H315 according to CLP and Xi; R38 according to DSD.

Comments received during public consultation

Three Member States provided comments on skin irritation/corrosion during the public consultation. Two agreed with the proposed classification while one questioned the use of in vitro studies to conclude on non-corrosion. The claim by the dossier submitter that corrosive properties decreased with increasing chain-length for straight chain organicnic acids was also questioned by this Member State.

Six industry commenters from the Fatty Acid Consortium (FAC) submitted an identical statement. For skin corrosion, the FAC agreed with the dossier submitter.

Assessment and comparison with the classification criteria

Since there is generally insufficient data on the individual organic acids, the dossier submitter used the available information on the homologues octanoic, nonanoic and decanonic acid, to derive a classification and labeling for the individual compounds. RAC supported this approach because the pK_a, values of the three acids are similar (octanoic acid, 4.89; nonanoic acid 4.96 and no pK_a for decanoic acid because it is a solid). These values are similar to the pK_a of 4.76 of acetic acid, which is corrosive to the skin (Category 1A, H314). However, the RAC noted that the pK_a and pH values are based on molarity. Since there are large differences in the molecular weights between acetic acid (60) and the three organic acids (octanoic acid 144, nonanoic acid 158, decanoic acid 172) their acidity per weight is lower than that of acetic acid. This explains the less clear irritating/corrosive effects of the three acids being considered here. Due to the close structural similarity and the very similar pK_a values RAC upported the weight of evidence approach of the dossier submitter.

The available information is briefly summarised below.

Assessment of Human patch tests (HPT)

A patch test on 72 human volunteers reported by Robinson et al. (1999) using octanoic and decanoic acid revealed at least mild irritation in 37 to 56% of the participants up to 1 hr and in 84 to 96% after up to 4 h exposure. For ethical reasons exposure was terminated at the first sign of irritation before 4 h of exposure.
In contrast to thedossier submitter, RAC did not see evidence from the York et al. (1996) study that decanoic acid produced strong responses in some individuals at 2 h. The report only states that as the concentration was increased, eventually 100% of the volunteers responded and that labelling with R38 was justified.

Irritation by nonanoic acid was also reported by Wahlberg (1983; 0.1 ml neat nonanoic acid repeatedly for 15 days on the forearm, 1 person).

The studies by Willis et al. 1988 and Wahlberg et al. (1985) continued exposure even after signs of irritation were noted. Willis et al. (1988) applied up to 80% nonanoic acid for 48 h to 42 healthy non-atopic male volunteers (not 70 as reported in the CLH report). In 28 volunteers exposed to an 80% solution, up to moderate skin reactions (erythema with oedema and papules) but no corrosion were observed. In a similar study, Wahlberg et al. (1985) reported skin irritation with increasing concentration but no corrosion. In this study up to 40% nonanoic acid was applied to 100 hospitalised patients with various skin diseases. At 20% and 40% nonanoic acid, all the 25 exposed patients reacted with skin irritation. The ED_{50} for irritation was about 6%.

Jirova et al. (2008) used the data from 25 compounds to compare the outcome of studies with the EpiDerm model applying 15 and 60 min exposure times and the 4h human patch test (HPT 0.2 g nonanoic and decanonic acid for 4 h, observation time up to 72 h) with data on rabbits. Whereas decanoic acid showed irritation in all three tests, nonanoic acid resulted in irritation from the EpiDerm and HPT test data, and borderline corrosion or irritation from the rabbit study. When compared with the 4h HPT results, the rabbit in vivo test provided 100% sensitivity (5/5), but only 50% specificity (10/20). The EpiDerm protocol with 15 min exposure corresponded better to the response seen in man – sensitivity 80% (4 of 5 irritants classified correctly), while the optimized EpiDerm protocol with 60 min exposure time reached higher concordance with the rabbit test.

The above authors concluded that although the rabbit test exhibited 100% sensitivity, but only 50% specificity, the rabbit test identifies irritants reliably, however 50% of non-irritants are wrongly labelled as irritants.

However, RAC noted that no information on the rabbit tests or on the reason for corrosion/irritation for nonanoic acid is provided. Through personal communication with thedossier submitter, the study authors were contacted and reported that the HPT on nonanoic and decanoic acids showed irritation after 4 h, not at shorter times of exposure

Based on the human patch test studies, RAC supported the conclusion of thedossier submitter that the three organic acids are at least skin irritants, but did not consider that the studies provide evidence for corrosive effects.

Assessment of animal and in vitro studies

The rabbit study reported by Jirova et al. (2008) could not be used to support classification because no information on the test procedure or details of the outcome were provided.
Smyth et al. (1962), using 5 albino rabbits exposed to 0.1 ml 100% octanoic or decanoic acid for 24 h, report severe irritation. Reversibility was not determined.

Van Otterdijk (2001), using 3 male rabbits exposed to 75 mg/cm^2 100% nonanoic acid for 4 h and observation up to 72 h, also reported severe irritation and (very) slight oedema, which had resolved within 15 days. Oedema could not be scored on days 3, 4 and/or 8 due to fissuring; scab formation and/or brown discolouration (sign of necrosis) of the treated skin was observed among all animals between days 1 and 8. Scabs, eschar formation and/or fissuring of the skin were noted on days 3, 4 and/or 8 among the animals. In addition, bald skin and scaliness were observed at the end of the observation period, at day 14 in all 3 animals.

According to CLP, corrosive reactions are typified as ulcers, bleeding, bloody scabs, and by the end of observation at 14 days, by discolouration due to blanching of the skin, complete areas of alopecia, and scars. Of these, only the alopecia at day 14 meets the criteria for corrosion, therefore thedossier submitter considered these effects borderline for classification as corrosive.

Irritation has also been observed in the acute dermal toxicity test in rats (25% decanoic acid for 24 h), which was reversible within 15 days (Talvioja, 2006). The acute dermal toxicity study in rats with 22% nonanoic acid for 24 h showed severe irritation (van Otterdijk, 2001). The erythema was not reversible in 3/10 animals within 15 days.

In an OECD TG 406 skin sensitisation test in Guinea pigs, 24 h exposure to nonanoic acid at concentrations above 50% was reported as severely irritating but with an oedema grade of 1 at 24 and 48 h. Reversibility was not investigated (Talvioja, 2006).

In a local lymph node assay (LLNA) in mice, 25 µl/ear of 70% decanoic acid applied 3 times in 3 consecutive days was mildly irritant, which did not reverse within 6 days (Weber et al., 2006).

Since thedossier submitter considered the findings as borderline to corrosion, they used the Toxtree QSAR evaluation of the three organic acids (which revealed irritating or corrosive to skin) and the in vitro rat skin corrosivity test on the basis of transcutaneous electrical resistance (TER), which indicated skin corrosion. However, the RAC concluded that the outcomes of these in vitro tests are overruled by the weight of evidence from the various in vivo tests, including the human data, which did not show corrosion.

Comparison with classification criteria

When tested in rabbits, guinea pigs and mice the three organic acids induced mild to severe skin irritation in a high percentage of the animals. When determined, there was reversibility within 15 days in the animal studies. Unfortunately, the reports do not provide information on the severity of the effects. Irritation was also seen in the HPT in most of the volunteers exposed up to 48 h at concentrations of 20% and higher.

The RAC noted that the evidence for skin corrosion of nonanoic acid is borderline. Since the available information on nonanoic acid does not clearly indicate skin corrosion and considering their similar pKa values, RAC does not consider that there is sufficient evidence to classify decanoic acid as corrosive to skin.
Based on a weight of evidence approach and in agreement with the dossier submitter, RAC concluded that decanoic acid should be considered as irritating to the skin and classified as Skin Irrit. 2 - H315 according to CLP (Xi; R38 according to DSD).

RAC evaluation of eye irritation

Summary of the Dossier submitter's proposal

No guideline-compliant studies assessing eye irritation or damage are available for decanoic acid. The CLH report included two older non-GLP studies using decanoic acid in rabbits. Smyth *et al.* (1962) attributes a score of 9 out of 10 for corneal opacity but reversibility is not assessed. Briggs et al. (1976) indicated corneal opacity and moderate conjunctivitis with no reversibility after 72 hours but assigned no scoring. Based on these observations and the severe skin irritating properties of decanoic acid, the dossier submitter proposes classification as Eye Dam. 1 – H318 according to CLP and R41 according to DSD.

Comments received during public consultation

Two Member States submitted comments agreeing with the proposed classification for eye effects. Six industry commenters from the Fatty Acid Consortium (FAC) submitted an identical statement arguing that the data from Briggs et al. (1976) and Smyth et al. (1962) should not be used for classification and reported that a new in vitro study will be commissioned to assess eye effects of decanoic acid. Another comment received from industry mentioned a Bovine Corneal Opacity and Permeability (BCOP) test conducted with decanoic acid, indicating non-corrosivity. The study was not however made available to the dossier submitter for assessment.

Assessment and comparison with the classification criteria

There are no guideline specific eye irritation studies on octanoic-, nonanoic-, or decanoic acid reported in the CLH dossiers. Due to the proposed Classification & Labelling of the three organic acids as irritants to the skin (see above) and the similar pK_a values of octanoic and nonanoic acid, the RAC used the information available on the individual compounds for the evaluation of all three organic acids.

Regarding octanoic and decanoic acid, two older, non-GLP compliant studies in rabbits (Smyth et al., 1962 and Briggs et al., 1976) were available to the DS. The Smyth et al. study in 5 rabbits per group resulted in grade 9 corneal effects , indicating risk for severe damage to the eye for both octanoic and decanoic acid. No information on the concentration or on the reversibility was provided. The Briggs et al. (1976) study revealed corneal opacity, with no reversibility up to 72 h. No information on the number of rabbits or on the concentrations of the test compounds was provided and no scoring was applied.

For octanoic acid, industry provided information from a study by Leoni and Riedel (2011) during the public consultation. In 2 out of 3 rabbits tested, lesions of the iris with a score equal to 1 were induced using 70% octanoic acid. The effects were fully reversible within 6 – 11 days. The test would result in classification as Eye Irrit. 2 – H319 at 70%. Thedossier submitter supported this proposal although the study was not made available to them. The RAC evaluated the Leoni and Riedel (2011) study. In accordance with the OECD TG 403 test guideline, 0.1 ml of 70% octanoic acid has been applied for 24 h to 3 rabbits. The animals were observed over 72 h and at 6, 9, and 11 days after dosing. Conjunctival redness, chemosis and discharge were observed in all animals with average scores of 1, 1.67 and 2. In two animals, lesions of the iris (average score 1 for both animals) and the cornea (average scores 1.33 and 0.67, respectively) were observed. At the end of the prolonged observation period of 9 days no corneal, iris or other lesions were seen in any of the animals. According to the CLP criteria, this corresponds to a classification as Eye Irrit. 2 – H319 (Xi; R36 according to DSD). This more recent study does not confirm the results of the older non-guideline studies.

During the public consultation, industry also referred to a Bovine Corneal Opacity and Permeability (BCOP) test for decanoic acid, which indicates non-corrosivity. The RAC evaluated this OECD TG 437 study and concluded that based on the criteria of the guideline a 20% dilution of decanoic acid was not corrosive or a severe irritant to the eye. The in vitro opacity score was 16.83 as compared to a score of ≥ 55.1 at which a substance is considered to be corrosive or a severe irritant.

For nonanoic acid no eye damage or eye irritation data are available.

Comparison with the criteria

The available information is inconsistent and does not allow a clear differentiation between irreversible and reversible effects on the eyes. The poorly described Smyth et al.(1962) study indicates that there were irreversible effects resulting from treatment with octanoic and decanoic acid, which is not supported by the study of Briggs et al. (1976) and the more recent study by Leoni and Riedel (2011) on octanoic acid, from which classification as Eye Irrit. 2, H313 at 70% could be considered. The study by Briggs et al. (1976) does not provide sufficient information to evaluate the irritating potencies of octanoic and decanoic acids.

Based on the data on octanoic and decanoic acid RAC concluded that classification as Eye Irrit. 2, H313 according to CLP (Xi; R36 according to DSD) for decanoic acid was warranted.

RAC evaluation of respiratory irritation

Summary of the Dossier submitter's proposal

The dossier submitter indicated that due to the strong skin and eye irritating properties of decanoic acid, it can be assumed that the substance has respiratory irritating properties as well. However, the available acute inhalation studies do not show sufficient evidence for respiratory tract irritation and the CLP Regulation requires classification as STOT SE 3 -H335 to be largely based on human respiratory data, which is not available for decanoic acid. Therefore, the dossier submitter proposed no classification for respiratory tract irritation.

Comments received during public consultation

One Member State commented during public consultation that respiratory tract irritation was reported in the Draft Assessment Report (DAR) for decanoic acid, in an acute inhalation study using a biocidal product containing decanoic acid. The member State requested that RAC conduct a detailed evaluation on the respiratory tract irritation potential of decanoic acid and that RAC consider classification as STOT-SE 3 – H335 (CLP) and Xi; R37 (DSD)

Assessment and comparison with the classification criteria

In the CLH report, no LC_{50} value for acute inhalation toxicity on octanoic acid is described. Exposure of rats to the saturated vapour for 4 h did not result in mortality.

Acute 4 h inhalation toxicity studies on nonanoic acid revealed LC_{50} values of > 5.3 and > 5.9 mg/L, and > 0.55 mg/L for the ammonium salt, which was the highest achievable concentration. In this study, no macroscopic pathological effects were observed. In another rat study the LD_{50} was > 1 mg/L without macroscopic pathological effects after 14 days of recovery.

Decanoic acid exposure to rats (the saturated vapour) for 4 and 8 h did not result in mortality. A 2 h exposure to an unknown species resulted in a LC_{50} of > 4.1 and > 5.5 mg/L.

These studies do not allow evaluation of respiratory tract irritation. Since the melting points and boiling points of the three organic acids are relatively high (octanoic acid: MP 16.7 °C, BP 239.7 °C; nonanoic acid: MP 12.5 °C, BP 254 °C; decanoic acid: MP 31.6 °C, BP 269 °C) a significant inhalation exposure, which may lead to respiratory irritation seems to be unlikely.

Based on the information on the three organic acids and considering their close structural and physical similarities, RAC concluded that there was insufficient evidence to support classification of decanoic acid as a respiratory irritant.

ENVIRONMENTAL HAZARD ASSESSMENT

RAC evaluation of environmental hazards

Summary of the Dossier submitter's proposal

The ecotoxicological tests on fish (for octanoic acid), crustaceans and algae (for decanoic acid) presented in the CLH report show that the lowest short term value is the ErC_{50} for algae (= 2 mg/L). Since the $L(E)C_{50}$ values are all above 1 mg/L, the dossier submitter concluded that the criterion for classification for acute aquatic hazard Category 1 (CLP) and R50 (DSD) are not fulfilled.

The dossier submitter considered decanoic acid as readily biodegradable and rapidly degradable since in a manometric respirometric test (OECD TG 301F), a mean degradation rate of 92% at the end of the 28-days exposure period was observed.

In the CAR for biocides, the calculated log Pow is 4.09 and the resulting calculated BCF on fish would be 598.

In relation to the long term aquatic hazard according to the 2nd ATP of the CLP Regulation, only long term data on algae (*Desmodesmus Subspicatus*) are available, these data provided a geometric mean NOEC of 0.57 mg/L (72 h growth inhibition test, presented in the CAR for biocides).

In the RCOM, the dossier submitter recalculated the NOEC for algae according to a new approach (described in the following section) and proposed a value of 0.249 mg/l.
For fish and crustaceans only, acute toxicity values (in the range of 10-100 mg/l) are available.
Based on the long term and acute toxicity values for the three trophic levels, in combination with rapid degradability, the dossier submitter proposed to classify decanoic acid as hazardous to the aquatic environment, chronic Category 3 - H412, according to CLP. Based on the values for aquatic acute toxicity (1 mg/L < ErC_{50} for algae = 2 mg/L $\leqslant$ 10 mg/L) and the log Kow ($\geqslant$ 3), the dossier submitter proposed to classify as R51/53 according to Directive 67/548/EEC (DSD).

Comments received during public consultation

During the public consultation, comments on hazards to the aquatic environment were received from four Member States Competent Authorities (MSCAs) and six companies.

Two MSCAs supported the classification proposal. Another MSCA requested clarification on which data the proposal is based and that Specific Concentration Limits (SCLs) should be added.
In response to this comment, the dossier submitter included in the RCOM a summary of all available acute and chronic ecotoxicity data from CARs on octanoic, nonanoic and decanoic acids and REACH registration dossiers on octanoic and nonanoic acids (see ECHA web site). In relation to the SCLs, the dossier submitter pointed out that no SCLs were needed since the substance was not classified as R50 or R50/53 (DSD) and also no M-factors ewre needed since the substance was not classified as aquatic acute 1 or aquatic chronic 1.

Another MSCA suggested that a wider set of ecotoxicity data relating to the analogues (heptanoic, octanoic and nonanoic acids) be considered, which are available in the REACH registration dossiers, in order to understand and validate the read-across to decanoic acid and to address some potentially conflicting data. In response to this comment, the dossier submitter stated that the available data on decanoic acid and the weight of evidence from other medium chain fatty acids confirm the proposed classification.

The six companies referred to a report of the Fatty Acids Consortium (FAC) and proposed no classification, on the basis of the general characteristics of fatty acids, being naturally occurring and ubiquitously present in the aquatic environment, where they are readily biodegraded by microorganisms. They underpinned their justification with the argument that the logPow was inappropriate as a predictor of bioaccumulative properties of fatty acids.

Moreover, they claimed that there were methodological deficiencies in the studies used to conclude on classification in the CLH report. They questioned the use of 72h-NOEC instead of 48h-NOEC in the algae test for decanoic acid under the Biocide Directive, as well as the use of measured concentrations. (In their view, fatty acids act as nutrient for algae. Since the applied amount is not lost from the system but becomes part of the cells, nominal concentrations should be used).

The FAC report proposed that the NOEC of 3.2 mg/L, which was obtained in a new algae (*Selenastrum capricornutum*) growth inhibition study on decanoic acid, should be considered. This value would warrant "no classification" according to the CLP regulation. Also, long term studies on aquatic invertebrates (daphnia) for decanoic acid have been conducted and test data were expected by October 2012.

The dossier submitter responded to this comment by supporting the classification as Aquatic Chronic 3 and describing the cause of the observed effects in the long term test on algae used for classification purposes and considering the NOEC values of the homologous substances. Moreover, the NOEC of this study was recalculated as the geometric mean from the measured concentrations at the beginning of the test and from half of the limit of quantification at all other measuring points. According to this new approach, the NOEC of this algae study was recalculated as 0.249 mg/l.

For the full set of comments and responses, see the response to comments document (RCOM) in Annex 2.

Assessment and comparison with the classification criteria

Degradation

Decanoic acid was readily biodegradable in an OECD TG 301F manometric respirometry test showing degradation of 91-92% at 28 days and of 79-80% within the 10 d window. Hydrolysis and photolytic degradation in water were excluded for decanoic acid because organic acids cannot be hydrolysed in the absence of further functional groups and it does not display chromophore properties at wavelengths above 290 nm.

Based on the available data, RAC agreed with the dossier submitter that decanoic acid should be considered **readily biodegradable** according to DSD and **rapidly degradable** according to CLP.

Bioaccumulation

No experimental log kow could be determined for decanoic acid, because the octanol /water coefficient cannot be accurately estimateded.

A calculated log Kow value of 4.09 has been summarized in the CLH report. This log Kow corresponds to an undissociated acid but at relevant environmental pHs, decanoic acid is found in a dissociated form (the pka value for decanoic acid in water is extrapolated from known pKa values of other alkyl homologues and is expected to be in the range from 4.89 to 5.03), and therefore, the log kow is expected to be lower. Nevertheless, decanoic acid is suspected to be a surface active substance (the value of surface tension is not available), and according to the Technical Guidance Document on Risk Assessment (EC 2003, part II, p. 24), for a substance of this type it may not be advisable to use an estimated or measured Kow values as a predictor for Koc (soil, sediment, suspended organic matter and sludge) and BCF (fish, worm), because the predictive value of log Kow for such estimations may be too low. Instead, for surfactants it may be appropriate to obtain measured Kp and BCF values.

For decanoic acid, there is no BCF available; however, in the REACH registration dossier for octanoic acid, there is an experimental BCF performed with sodium laurate (dodecanoic acid), which can be used to provide some information for decanoic acid. The measured BCF value for dodecanoic acid is 255 L/kg, but it is based on total radio-labelled residues and therefore this is an overestimate. Nevertheless, according to the Guidance on the application of the CLP criteria (p.

506), if an experimental BCF based on the parent compound is not available, for classification purposes, the BCF based on radio-labelled residues can be used.

The test shows some deficiencies, such as the depuration phase was not determined, the fish were only sampled at the end of the exposure and that the study was not GLP compliant, however, this test can indicate the bioaccumulation potential of similar substances and therefore it can be used as supportive information.

In conclusion, since the log Kow may be an unreliable predictor of bioconcentration potential for this substance, it is not appropriate to compare it with the classification criteria. No measured BCF data are available for decanoic acid itself. The C_{12} analogue dodecanoic acid is more hydrophobic than decanoic acid, so a direct application of its measured fish BCF is likely to be a worst case approach. The implication in the absence of any further evidence is that the BCF of decanoic acid is below 500 L/kg, but it cannot be ruled out that the BCF is above 100 L/kg.

Aquatic toxicity

A summary of ecotoxicological data of different, structurally similar organic acids has been summarised in the additional key elements section, table 1.

As can be seen in this table, when the toxicity to fish and daphnia is evaluated, the expected relationship between the toxicity and hydrophobicity of the acids is observed. Since water/fat solubility is related to the chain-length of the acids, their toxicities follow the order: dodecanoic acid > decanoic acid > nonanoic acid > octanoic acid. However regarding the toxicity to algae, which is clearly the most sensitive taxonomic group, some data are too inconsistent to enable a classification to be established.

Three different algae tests were included in the report, one performed with nonanoic acid gave a NOEC of 0.57 mg/L (Competent Authority Report, CAR, of biocides), one more performed with decanoic acid gave a NOEC of 0.21 mg/l (CAR) and finally another one with octanoic acid gave a NOEC of 0.07 mg/L (REACH registration dossier). Information on dodecanoic acid was also included in order to follow the trend of the toxicity, and the NOEC for algae was 0.079 mg/L (CAR). All these values were based on mean measured concentrations.

The tests for nonanoic, decanoic and dodecanoic acids were performed with the same algae species (*Desmodesmus Subspicatus*) and for octanoic acid the selected algae species was *Pseudokirchnerella Subcapitata*, these two species are recommended by the OECD TG 201 guideline. As can be seen in the results, *Pseudokirchnerella subcapitata* appears to be the most sensitive species and therefore octanoic acid the most toxic compound. This result from the REACH registration dossier is not consistent with the results obtained in daphnia and fish or with the trend observed in the algae tests carried out on the substances in the group. When this test is not considered, toxicity appears to increase with hydrophobicity as would be expected.

Furthermore, there are some deficiencies in the above tests, such as the inconsistency in dose-responsiveness at the lowest concentrations, the rapid loss of the test concentration and the fact that the highest effect is observed at 24 hours. Therefore, taking into account that the reliability of this test cannot fully be confirmed and that this test is not consistent with the results of the other taxonomic groups, it should not be used for classification purposes.
For decanoic acid there is an algae test available with *Desmodesmus subspicatus*, the same species used for nonanoic acid test, which can be used to classify.

As the test substance was not detectable at the end of the algae tests performed with nonanoic and decanoic acids, the 48 h time interval becomes relevant. However, in the 72- hour algal growth inhibition test with decanoic acid, the following validity criterion given in OECD TG guideline 201 is not fulfilled: "The test period may be shortened to at least 48 hours to maintain unlimited, exponential growth during the test as long as the minimum multiplication factor of 16 is reached". In case of the algae test with decanoic acid, the multiplication factor is only approximately 10. Therefore, the total test duration of 72 h has to be used for effect assessment and to estimate chronic effects (by using a concentration equal to half of the limit of quantification

when the test substance is not detectable). For decanoic acid it is not possible to check it due to the minimal data provided.

There is a rapid loss of the test concentrations in the tests with nonanoic, decanoic and dodecanoic acids; this rapid loss also appears in fish and daphnia studies (semi-static tests), as well as in the algal tests without algae for nonanoic and dodecanoic acids. Furthermore, it is necessary to take into account that decanoic acid together with octanoic and nonanoic acids, are surface active substances and the critical micelle concentration is not mentioned in the dossier; so the presence of micelles and adsorption to hard surfaces could partly explain the technical difficulties associated with measuring the actual concentrations of these acids.

According to the OECD TG 201, the use of nominal concentrations would be appropriate when a decrease in concentration of the test substance in the course of the test is not accompanied by a decrease in growth inhibition. In the algae test performed with decanoic acid it is observed that at 72h the growth inhibition is lower than at 48h when the concentration was higher. Therefore, at least for this test, the criterion for using nominal concentrations is not met.

Moreover, under the Biocides Directive, the acute and chronic algae toxicity was based on mean measured concentrations. Taking into account the deficiencies of the test submitted under REACH registration for octanoic acid and the justified use of measured concentrations in the algae tests conducted with decanoic acid, the classification is as follows.

Under CLP, the acute aquatic toxicity is based on EC_{50} values, and for decanoic acid these values are >1 mg/l, therefore decanoic acid does not meet the criteria for classification for aquatic acute toxicity. This value is consistent with the acute toxicity of other structurally similar compounds (octanoic and nonanoic acid), which also have LC_{50} values higher than 1 mg/L.

Regarding chronic toxicity, the most sensitive species is the algae (*Desmodesmus subspicatus)* with a NOErC of 0.25 mg/L. Taking into account this value and its rapid degradation, decanoic acid can be classified as **Chronic category 3 (H412)** according to **CLP**. Although there are no chronic tests in fish, the surrogate approach is not relevant since decanoic acid is readily biodegradable and has a fish BCF <500 L/kg and therefore leads to no classification.

Considering the **DSD classification**, the ErC_{50} value for algae is 2 mg/L and although the substance is readily biodegradable, a BCF value > 100 L/kg cannot be ruled out, therefore classification as R51/R53 is therefore justified.

ANNEXES:

Annex 1 Background Document (BD) gives the detailed scientific grounds for the opinion. The BD is based on the CLH report prepared by the dossier submitter; the evaluation performed by RAC is contained in RAC boxes.

Annex 2 Comments received on the CLH report, response to comments provided by the dossier submitter and rapporteurs' comments (excl. confidential information).

REFERENCES:

Leoni, A-L. and Riedel, W. (2011). Acute Eye Irritation/Corrosion with Octanoic Acid. Testing laboratory: BSL Bioservice, Planegg, Germany. Report no.: 112747. Owner company: FATAC Ltd., Gloucestershire, England. Report date: 2011-10-21