EUROPEAN CHEMICALS AGENCY

Helsinki, 27 May 2020

Addressees
Registrants of JS_61789-32-0 listed in the last Appendix of this decision

Date of submission for the jointly submitted dossier subject of this decision
05/10/2018

Registered substance subject to this decision, hereafter 'the Substance'
Substance name: Fatty acids, coco, 2-sulfoethyl esters, sodium salts
EC number: 263-052-5
CAS number: 61789-32-0

Decision number: [Please refer to the REACH-IT message which delivered this communication (in format CCH-D-XXXXXXXXXX-XX-XX/D)]

DECISION ON A COMPLIANCE CHECK

Based on Article 41 of Regulation (EC) No 1907/2006 (REACH), ECHA requests that you submit the information listed below by the deadline of ***4 December 2023***.

A. Requirements applicable to all the Registrants subject to Annex VII of REACH

1. In vitro gene mutation study in bacteria (Annex VII, Section 8.4.1.; test method EU B.13/14. / OECD TG 471) with the Substance using one of the following strains: *E. coli* WP2 uvrA, or *E. coli* WP2 uvrA (pKM101), or *S. typhimurium* TA102

2. Short-term toxicity testing on aquatic invertebrates (Annex VII, Section 9.1.1.; test method: EU C.2./OECD TG 202) with the Substance

3. Growth inhibition study aquatic plants (Annex VII, Section 9.1.2., test method: EU C.1./OECD TG 201) with the Substance

4. Ready biodegradation (Annex VII, Section 9.2.1.1.; test method OECD TG 301B/C/D/F or OECD TG 310) with the Substance

B. Requirements applicable to all the Registrants subject to Annex VIII of REACH

1. Screening for reproductive/developmental toxicity (Annex VIII, Section 8.7.1.; test method OECD 421/422) in rats, oral route with the Substance

2. Short-term toxicity testing on fish (Annex VIII, Section 9.1.3.; test method OECD TG 203) with the Substance

3. Hydrolysis as a function of pH (Annex VIII, Section 9.2.2.1., test method: OECD TG 111) with the Substance

4. Adsorption/desorption screening (Annex VIII, Section 9.3.1., test method: OECD TG 106) with the Substance

C. Requirements applicable to all the Registrants subject to Annex IX of REACH

1. Sub-chronic toxicity study (90-day), oral route (Annex IX, Section 8.6.2.; test method OECD TG 408) in rats with the Substance

2. Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.; test method OECD TG 414) in a first species (rat or rabbit), oral route with the Substance

3. Long-term toxicity testing on aquatic invertebrates (Annex IX, Section 9.1.5.; test method: EU C.20./OECD TG 211) with the Substance

4. Long-term toxicity testing on fish (Annex IX, Section 9.1.6.1.; test method OECD TG 210) with the Substance

5. Simulation testing on ultimate degradation in surface water (Annex IX, Section 9.2.1.2.; test method: EU C.25./OECD TG 309) at a temperature of 12 °C with the Substance

6. Sediment simulation testing (Annex IX, Section 9.2.1.4.; test method: EU C.24./OECD TG 308) at a temperature of 12 °C with the Substance

7. Bioaccumulation in aquatic species (Annex IX, Section 9.3.2; test method: OECD TG 305) with the Substance

Conditions to comply with the requests

Each addressee of this decision is bound by the requests for information corresponding to the REACH Annexes applicable to their own registered tonnage of the Substance at the time of evaluation of the jointly submitted dossier.

To identify your legal obligations, please refer to the following:

- you have to comply with the requirements of Annex VII of REACH, if you have registered a substance at 1-10 tonnes per annum (tpa), or as a transported isolated intermediate in quantity above 1000 tpa;
- you have to comply with the requirements of Annexes VII and VIII of REACH, if you have registered a substance at 10-100 tpa;
- you have to comply with the requirements of Annexes VII, VIII and IX of REACH, if you have registered a substance at 100-1000 tpa.

Registrants are only required to share the costs of information that they must submit to fulfil the information requirements for their registration.

The Appendix on general considerations addresses issues relevant for several requests while the other Appendices state the reasons for the requests for information to fulfil the requirements set out in the respective Annexes of REACH.

The Appendix entitled Observations and technical guidance addresses the generic approach for the selection and reporting of the test material used to perform the required studies and provides generic recommendations and references to ECHA guidance and other reference documents.

The studies relating to biodegradation and bioaccumulation (requests A.4 and C.5 to C.7) are necessary for the PBT assessment. However, to determine the testing needed to reach the conclusion on the persistency and bioaccumulation of the Substance, you should consider the sequence in which these tests are performed and other conditions described in Section

Strategy for the PBT/vPvB assessment of Appendix E.

You must submit the information requested in this decision by the deadline indicated above in an updated registration dossier and also update the chemical safety report, where relevant, including any changes to classification and labelling, based on the newly generated information. The timeline has been set to allow for sequential testing where relevant.

Appeal

This decision can be appealed to the Board of Appeal of ECHA within three months of its notification. An appeal, together with the grounds thereof, has to be submitted to ECHA in writing. An appeal has suspensive effect and is subject to a fee. Further details are described under: http://echa.europa.eu/regulations/appeals.

Approved[1] under the authority of Christel Schilliger-Musset, Director of Hazard Assessment

[1] As this is an electronic document, it is not physically signed. This communication has been approved according to ECHA's internal decision-approval process.

Appendix on general considerations

(i) Assessment of the Grouping of substances and read-across approach, in light of the requirements of Annex XI, Section 1.5.

You seek to adapt the following standard information requirements listed below by applying read-across approaches in accordance with Annex XI, Section 1.5:

- Screening for reproductive/developmental toxicity (Annex VIII, Section 8.7.1.)
- Sub-chronic toxicity study (90-day), (Annex IX, Section 8.6.2.)
- Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.)
- Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.)
- Adsorption/desorption screening (Annex VIII, Section 9.3.1.)

ECHA has considered the scientific and regulatory validity of your read-across approaches in general before assessing the specific standard information requirements in the following appendices.

Grouping of substances and read-across approach

Annex XI, Section 1.5. specifies two conditions which must be fulfilled whenever a read-across approach is used. Firstly, there needs to be structural similarity between substances which results in a likelihood that the substances have similar physicochemical, toxicological and ecotoxicological properties so that the substances may be considered as a group or category. Secondly, it is required that the relevant properties of a substance within the group may be predicted from data for reference substance(s) within the group.

Additional information on what is necessary when justifying a read-across approach can be found in the ECHA Guidance R.6 and related documents.

- You have provided a read-across justification document in IUCLID Section 13.

A. Predictions for toxicological properties

You provide the following reasoning for the prediction of toxicological properties:

The Substance and Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium salts are chemically very similar and are expected to show similar physico-chemical properties:

- "[The source substance] *contains the same functional groups, but differs in the fatty acid alkyl chain length*". You provide a typical composition of the Substance and of the analogue substance. This information was obtained from the analytical monitoring of exposure concentrations in the test medium of a growth inhibition study on algae.
- "*QSAR (US EPA EPISUITE) modelling of physic-chemical properties for the pure constituents show a trend of increasing melting point, boiling point and a decreasing vapour pressure and water solubility. These values calculated for single constituents show that it is reasonable to assume a trend in the direction indicated.*"

"*Read across is also performed from Sodium 2-hydroxyethane sulfonate, EC no.: 216-343-6. This chemical is used in the manufacture, but is also formed during metabolism in the human body, as demonstrated in the toxicokinetic section, CSR section 5.1.*"

The manufacturing process is similar:
"*The Isethionate source chemicals are of the same structure, and produced in the same way, but with variation in the alkyl chain length.*"

The Substance and Dodecanoic acid, 2-sulfoethyl ester, sodium salt (EC no. 230-949-8 / CAS no. 7381-01-3) are expected to be subject to similar (bio)transformation and the effects of (bio)transformation products are expected to be either similar or non-relevant:

- "*The Isethionate substances have a similar structure, and toxicokinetic data of Dodecanoic acid, 2-sulfoethyl ester, sodium salt show that breaking of the isethionate/laurate ester bond and oxidation of the resultant lauric acid is the major route of metabolism. The other product produced by hydrolysis of the ester bond would be sodium isethionate. Since no systemic toxicity is expected from the fatty acid part, read across is justified to the sodium isethionate.*"

ECHA understands that you predict the toxicological properties of the Substance using a read-across hypothesis which is based on the similar structure and on the formation of common (bio)transformation products. The properties of your Substance are predicted to be quantitatively equal to those of the source substance.

You intend to predict the properties of the Substance from information obtained from the following source substances:

- Sodium 2-hydroxyethanesulfonate with EC no. 216-343-6 for Sub-chronic toxicity study (90-day), (Annex IX, Section 8.6.2.); [redacted] (2009)

- Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium salts/ Milled SLI (76) with EC no. 287-024-7 for:
  - Screening for reproductive/developmental toxicity (Annex VIII, Section 8.7.1.); [redacted] (2008).
  - Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.); [redacted] (2008).
- ^{14}C radiolabelled sodium lauryl isethionate (SLI) and sodium stearyl isethionate (SSI) for Toxicokinetics (Annex VIII, Section 8.8.1.)

Concerning the predictions of toxicological properties based on the source substances identified above, ECHA notes the following shortcomings:

1) *Characterisation of the test materials used in the studies on the source substances*

   Annex XI, Section 1.5 of the REACH Regulation provides that "*substances whose physicochemical, toxicological and ecotoxicological properties are likely to be similar or follow a regular pattern as a result of chemical similarity may be considered as group.*"

   According to the ECHA Guidance, "*the purity and impurity profiles of the substance and the structural analogue need to be assessed*", and "*the extent to which differences in the purity and impurities are likely to influence the overall toxicity needs to be addressed, and where technically possible, excluded*". The purity profile and composition can influence the overall toxicity/properties of the Substance and of the source substance(s).[2] Therefore, qualitative and quantitative information on the compositions of the Substance and of the source substance(s) should be provided to

[2] Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of Chemicals, Section R.6.2.3.1

allow assessment whether the attempted predictions are compromised by the composition and/or impurities.

Furthermore, whenever the Substance and/or the source substances) are UVCB (Unknown or Variable composition, Complex reaction products or of Biological materials) substances qualitative compositional information of the individual constituents of the category members needs to be provided; as well as quantitative characterisation in the form of information on the concentration of the individual constituents of these substances; to the extent that this is measurable (ECHA Guidance R.6, Section R.6.2.5.5).

In your read-across justification document you report a typical composition for the source substance Milled SLI (76) based on *"based on measured total concentration in algae study"* in the test medium at the start of the experiment (t = 0h). In the algae study you describe the test material as *"SLI (76) stripped"* with Lot/batch No. S2849001. The test material used in the studies by ([redacted] 2008) is described as *"Milled SLI (76)"*. No information on purity or C-chain length distribution is reported for this source substance or for the source substances SLI and SSI used to generate the toxicokinetic data.

The quantitative information on the source substance Milled SLI (76) refers to the constituents that were dissolved in the test medium used in an algal growth inhibition study. It may be expected that the constituents of this analogue substance may have varying water solubility and adsorptive properties. Therefore the data generated may not provide an adequate description of the test substance itself but only of the constituents that were dissolved in the test medium. You have not provided compositional information on the test materials used to conduct the toxicological testing for the reproductive toxicity endpoints and toxicokinetics. Without adequate compositional information, no qualitative or quantitative comparative assessment of the compositions of the Substance and of the source substance can be completed. Therefore, ECHA considers that it is not possible to assess whether the attempted predictions are compromised by the composition of the source substance.

In your comments on the draft decision you indicate that *"Specific attention will be given in description of the substance identification, including explanation of the moving away from chemical name that historically denoted the coco source of the fatty alkyl chains (i.e. CAS no. 61789-32-0, Fatty acids, coco, 2-sulfoethyl esters, sodium salts) to a generic chemical name that describe the chain-length distribution (i.e. CAS no. 85408-62-4, Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium salts). Nowadays the origin of the alkyl chains can be variable, involving mixing of distilled fractions of various vegetable sources leading to similar chain length distribution as in coco."*

ECHA notes your intention to clarify the identify of the Substance and more specifically the fatty alkyl chain source. As explained above adequate compositional information on both the Substance and the source substances used in the tests is required to enable read across.

2) *Read-across hypothesis contradicted by existing data*

As indicated above, your read-across hypothesis is also based on the (bio)transformation of the Substance and of the source substances to a common compound (i.e. sodium isethionate used in your read-across as a source chemical for the 90-d study). In this context, information characterising the rate and extent of the

hydrolysis of the Substance and of the source substances is necessary to confirm the similar and rapid formation of the proposed common hydrolysis product and to demonstrate that the impact of the exposure to the parent compounds is negligible.

In that respect you explain that based on the data obtained with Dodecanoic acid, 2-sulfoethyl ester, sodium salt, the Substance and source substances are expected to undergo the same, rapid biotransformations *in vivo* to yield two types of hydrolysis products: the first being straight chain fatty acids (C8 to C18) and the second sodium isethionate.

You have provided a hydrolysis study in artificial fluids (i.e. simulated gastric fluid, simulated intestinal fluid & porcine liver esterase) with ^{14}C radiolabelled sodium lauryl isethionate (SLI) and sodium stearyl isethionate (SSI). You report that after 6 hours:

- SLI and SSI showed respectively 30% and 40% degradation in gastric fluid,
- SLI showed 10% degradation while SSI was stable in intestinal fluid, and
- SLI was almost completely degraded in porcine liver esterase while SSI only showed 20% degradation

However, the data you submitted does not support your claim that the Substance and source substances undergo the same, rapid biotransformations *in vivo*. The data rather show that there is significant exposure to the parent substance and that the two source substances used in these studies have different degradation behaviour in similar artificial fluids. This contradicts your read-across hypothesis that the target and source substances undergo the same, rapid biotransformations in vivo. Therefore, you have not demonstrated and justified that the properties of the source substances and of the Substance are likely to be similar despite the observation of these differences. Furthermore, you did not demonstrate the relevance of the data obtained with SLI and SSI for the Substance and source substances (e.g. SLI constitutes up to 44% of the target and 25% of the source Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium salts).

B. Predictions for ecotoxicological properties

i. Aquatic toxicity

You have provided the following reasoning for the prediction of aquatic toxicity: "*The toxicity to aquatic organisms is expected to increase with increasing alkyl chain length, which is also substantiated by modelling with ECOSAR 1.00 (US EPA)*". You provide a table showing the results of ECOSAR predictions (based on predicted log Kow) for short-term toxicity to aquatic invertebrates and fish and for growth inhibition to algae for fatty ester sulfonates ranging from C8 to C18 which you consider supportive of your hypothesis. You conclude that Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium salts "*can be considered to be a worst case*" to predict the ecotoxicological properties of the Substance.

ECHA understands that you predict the properties of the Substance using a read-across hypothesis which assumes that different compounds have the same type of effects. The properties of your Substance are predicted based on a based on a worst-case approach.

You intend to predict the properties of the Substance from information obtained from the source substance Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium salts with EC no. 287-024-7, which is used as a source substance for Growth inhibition study aquatic plants (Annex VII, Section 9.1.2).

ECHA notes the following shortcoming with regards to prediction of aquatic toxicity:

1) Characterisation of the source substances

As explained under section Predictions of toxicological properties, as you have not provided adequate compositional information, no qualitative or quantitative comparative assessment of the compositions of the Substance and of the source substance can be completed. Therefore, ECHA considers that it is not possible to assess whether the attempted predictions are compromised by the composition of the source substance.

In your comments on the draft decision you indicate that *"Specific attention will be given in description of the substance identification, including explanation of the moving away from chemical name that historically denoted the coco source of the fatty alkyl chains (i.e. CAS no. 61789-32-0, Fatty acids, coco, 2-sulfoethyl esters, sodium salts) to a generic chemical name that describe the chain-length distribution (i.e. CAS no. 85408-62-4, Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium salts). Nowadays the origin of the alkyl chains can be variable, involving mixing of distilled fractions of various vegetable sources leading to similar chain length distribution as in coco."*

ECHA notes your intention to clarify the identify of the Substance and more specifically the fatty alkyl chain source. As explained above adequate compositional information on both the Substance and the source substances used in the tests is required to enable read across.

2) Adequacy and reliability of the source studies

According to Annex XI, Section 1.5., if the grouping concept is applied then in all cases the results to be read across should have adequate and reliable coverage of the key parameters addressed in the corresponding test method referred to in Article 13(3).

However, none of the following studies were performed according to the testing specifications set out in the corresponding OECD TG:

- [redacted] (2008) used to cover the requirement for a growth inhibition study to algae and cyanobacteria;
- [redacted] (1985) used to cover the requirement for a growth inhibition study to algae and cyanobacteria.

Therefore these studies do not provide an adequate coverage of the key parameters foreseen to be investigated in the corresponding test method. The specific reasons are explained further below under the information requirement for a growth inhibition study to algae and cyanobacteria.

3) Use of QSAR data as supporting information to substantiate worst-case consideration

You have provided QSAR data on relevant constituents of the source and target substances in order to substantiate your read-across hypothesis which is based on the assumption that the source substance Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium salts with EC no. 287-024-7 constitutes a worst-case for the prediction of the property under consideration.

We have first assessed the validity of your QSAR information before considering whether it substantiates your worst case hypothesis.

A. Absence of QSAR documentation

Annex XI, Section 1.3. states that results obtained from valid QSAR models may be used instead of testing when the following cumulative conditions are met:

1. results are derived from a QSAR model whose scientific validity has been established;
2. the substance falls within the applicability domain of the QSAR model;
3. adequate and reliable documentation of the applied method is provided; and
4. the results are adequate for classification and labelling and/or risk assessment.

According to ECHA's Practical guide "How to use and report (Q)SARs", section 3.4, a QSAR Model Reporting Format (QMRF) and a QSAR Prediction Reporting Format (QPRF) are required to establish the scientific validity of the model, to verify that the Substance falls within the applicability domain of the model, and to assess the adequacy of the prediction for the purposes of classification and labelling.

You have provided ECOSAR 1.00 predictions for relevant constituents of the source and target substances showing an increasing trend in aquatic toxicity with alkyl chain length. The predictions also indicate that above C16 the predicted value may exceed the solubility limit.

However, you have not provided any documentation for the QSAR prediction. In particular, you have not included a QMRF and/or a QPRF in your technical dossier.

Therefore, ECHA cannot establish whether the model is scientifically valid, whether the Substance falls within the applicability domain of the model, and whether the results are adequate for classification and labelling and/or risk assessment.

B. Your worst case hypothesis

Your read-across hypothesis is based on the assumption that the source substance constitutes a worst-case for the prediction of the property under consideration. In this context, relevant, reliable and adequate information allowing a comparison of the properties of the Substance and of the source substance is necessary to confirm a conservative prediction of the properties of the Substance from the data on the source substance.

The QSAR data you have provided is not considered adequate as explained above so ECHA cannot compare the properties of the Substance and the source substance.

Additionally, the information you have provided suggests that constituents with long alkyl chains (above C16) may not cause toxicity up to their solubility limit. You also indicate that the source substance might contain higher amounts of C16 and C18 constituents when compared to the Substance. You have not explained the impact of this on your worst case hypothesis.

Consequently, you have not established that the source substance constitutes a worst-case for the prediction of the property under consideration.

ii. Adsorption/desorption

You have provided the following reasoning for the prediction of Adsorption/desorption:
"*Results from an adsorption-desorption study using Dodecanoic acid, 2-sulfoethyl ester, sodium salt has been used. Since this is the main constituent of Fatty acids, coco, 2-sulfoethyl esters, sodium salts read across is considered justified*".

ECHA understands that you predict the properties of the Substance using a read-across hypothesis which assumes that different compounds have similar properties. The properties of your Substance are predicted to be quantitatively equal to those of the source substance.

You intend to predict the properties of the Substance from information obtained from the source substance Dodecanoic acid, 2-sulfoethyl ester, sodium salt (EC no. 230-949-8 / CAS no. 7381-01-3), which is used as a source substance for Adsorption/desorption screening (Annex VIII, Section 9.3.1.); Corral and Brands (2009).

ECHA notes the following shortcomings with regards to your prediction on adsorption/desorption screening:

1) Adequacy and reliability of source study

According to Annex XI, Section 1.5., if the grouping concept is applied then in all cases the results to be read across should have adequate and reliable coverage of the key parameters addressed in the corresponding test method referred to in Article 13(3).

The study you have provided ([redacted] 2009) was not performed according to the testing specifications set out in the corresponding OECD TG. The specific reasons are explained further below under the information requirement for Adsorption/desorption screening.

2) Missing supporting information to compare properties of the substances

As indicated above, your read-across hypothesis is based on the assumption that the structurally similar substances have similar fate properties. In this context, relevant, reliable and adequate information allowing to compare the properties of the Substance and of the source substance(s) is necessary. Such information can be obtained, for example, from bridging studies of comparable design and duration for the Substance and of the source substance(s).

In your technical dossier you have provided an adsorption/desorption screening study on Dodecanoic acid, 2-sulfoethyl ester, sodium salt (EC no. 230-949-8 / CAS no. 7381-01-3). You have not provided any study on the Substance.

However as already explained under issue 1) above, you have not provided any reliable studies on the selected source substance. In addition, your dossier does not include any relevant information on the Substance. Therefore, the data set reported in the technical dossier does not include such relevant, reliable and adequate information for the Substance and of the source substance(s) to support your read-across hypothesis.

C. Conclusions on the read-across approach

As explained above, you have not yet established that relevant properties of the Substance can be predicted from data on the analogue substance. Therefore, your adaptation does not comply with the general rules of adaptation as set out in Annex XI, Section 1.5. and your grouping and read-across approach is rejected.

(ii) Strategy for aquatic testing

Due to lack of reliable acute aquatic toxicity data on invertebrates or on fish it is not possible to determine the sensitivity of species. Therefore, the Integrated testing strategy (ITS) outlined in ECHA Guidance, Chapter R7b (Section R.7.8.5 including Figure R.7.8-4), is not applicable and both the long-term studies on invertebrates and on fish are requested.

Appendix A: Reasons for the requests to comply with Annex VII of REACH

Under Articles 10(a) and 12(1) of REACH, a technical dossier registered at 1 to 10 tonnes or more per year must contain, as a minimum, the information specified in Annex VII to REACH.

1. In vitro gene mutation study in bacteria (Annex VII, Section 8.4.1.)

An *In vitro* gene mutation study in bacteria is a standard information requirement in Annex VII to REACH.

You have provided in your dossier:

i. a key study by [redacted] (1991) corresponding to a bacterial reverse mutation assay performed according to OECD TG 471 with the Substance.
ii. a key study by [redacted] (1984) corresponding to a bacterial reverse mutation assay performed according to OECD TG 471 with the Substance.
iii. a key study by [redacted] (1994) corresponding to a bacterial reverse mutation assay performed according to OECD TG 471 with the Substance.

We have assessed this information and identified the following issue(s):

To fulfil the information requirement, the study has to meet the requirements of OECD TG 471 (1997). The key parameter(s) of this test guideline include that the test must be performed with 5 strains: four strains of *S. typhimurium* (TA98; TA100; TA1535; TA1537 or TA97a or TA97) and one strain which is either *S. typhimurium* TA102 or *E. coli* WP2 uvrA or *E. coli* WP2 uvrA (pKM101)

You provided information on the following strains: *S. typhimurium* TA 98, TA 100, TA 1535, TA 1537, TA 1538.

The reported data for the studies you have provided did not include the required fifth strain. *S. thyphimurium* TA102 or *E. coli* WP2 uvrA or *E. coli* WP2 uvrA (pKM101).

The information provided does not cover key parameter(s) required by OECD TG 471. Therefore, the information requirement is not fulfilled.

In your comments on the draft decision you agreed that the provided studies cover only four strains instead of the required 5 strains. You stated that based on the structure of the Substance there are no cross-linking properties, because the structure does not have reactive functional groups, which could act as a cross-linking agent. In addition, you stated that the substance does not have oxidising properties and it is not a hydrazine derivative.

Regarding the missing 5th strain, it does not detect exclusively oxidising mutagens, cross-linking agents and hydrazines, it can also demonstrate the effect of other types of substances. In addition the 5th strain detects mutations at AT base pairs (while the four standard *S. typhimurium* strains detect mutations at GC base pairs)[3,.4, 5,]

[3]Wilcox, P., Naidoo, A., Wedd, D. J. and Gatehouse, D. G. (1990). Comparison of Salmonella typhimurium TA 102 with Escherichia coli WP2 Tester strains. Mutagenesis, 5, 285-291. (NB: it is the reference 19 mentioned in paragraph 13 of OECD TG 471 of 1997.

[4] Gatehouse DG, Haworth S, Cebula T, Gocke E, Kier L, Matsushima T, Melcion C, Nohmi T, Ohta T, Venitt S, Zeiger E (1994). Recommendations for the performance of bacterial mutation assays. Mutat Res. 1994 Jun;312(3):217-33.

[5] Levin DE, ... Ames B (1982) A new Salmonella tester strain (TA102) with AT base pairs at the site of mutation detects oxidative mutagens. Proc. Nadl Acad. Sci. USA, Genetics, Vol. 79, pp. 7445-744

You provide information on structural alerts from QSAR Toolbox v 4.3 and conclude that no alert was found for bacterial mutagenicity. There was a micronucleus alert but you argue that it is not predictive for bacterial mutagenicity.

You also provided information obtained with DEREK (Derek Nexus v.6.0.1) which classifies this structure as Inactive for 'Mutagenicity in vitro in bacterium', with "no misclassified or unclassified features".

However, structural alerts cannot address adequately the five strains of the Ames test, because the tools uses aggregated Ames mutagenicity data, which is converted to YES/NO format. A common problem with all QSAR Toolbox profilers is that the endpoint is broadly defined (i.e. alerts for Ames test), but details on strains and data aggregation are missing. The structural boundaries used to define the chemical classes, or alerting on groups responsible for binding with biological macromolecules, represent structural functionalities in the molecule which could be used for building chemical categories for subsequent data gap filling but are not recommended to be used directly for prediction purposes (as structure-activity relationships, SARs). In addition, the yes/no results do not specify or address the different bacterial strains.

You also refer to paragraph 6 of OECD 471 which indicate when the bacterial reverse mutation test may not be appropriate. However, you did not provide any information why your substance falls under those examples considered in the test guideline.

Therefore, the information provided still does not fulfill the information requirement for this endpoint.

Study design

To fulfil the information requirement for the Substance, the *in vitro* gene mutation study in bacteria (OECD TG 471) should be performed using one of the following strains: E. coli WP2 uvrA, or E. coli WP2 uvrA (pKM101), or S. typhimurium TA102.

2. Short-term toxicity testing on aquatic invertebrates (Annex VII, Section 9.1.1.)

Short-term toxicity testing on aquatic invertebrates is a standard information requirement in Annex VII to REACH.

You have provided in your dossier:

(i) a key study by [redacted] (2003) corresponding to a short-term toxicity study to aquatic invertebrates performed according to OECD TG 202 with the Substance;
(ii) a supporting study by [redacted] (1984) corresponding to a short-term toxicity study to aquatic invertebrates performed similar to OECD TG 202 with the Substance;
(iii) a supporting study by [redacted] (1992) corresponding to a short-term toxicity study to aquatic invertebrates performed according to OECD TG 202 with the Substance;
(iv) a supporting study by [redacted] (1994) corresponding to a short-term toxicity study to aquatic invertebrates performed according to DIN 38412 with the Substance.

We have assessed this information and identified the following issue:

Tests on substances must be conducted in accordance with the OECD test guidelines or

another internationally recognised international test method (Article 13(3) of REACH). OECD TG 202 requires that all the following conditions are met (among others):

- an adequate description of the test material including purity, the presence (or not) of any co-formulant, the relative abundance of unreacted material(s), the distribution of the C-chain length for the active substance) is provided,
- an analytical monitoring of exposure concentrations is provided (including method description and results),
- an adequate description of the test medium is provided (including pH, hardness, Ca/Mg ratio, Na/K ratio, alkalinity, conductivity, DOC and suspended solid content),
- the spacing factor between test concentrations must not exceed 2.2.

For study (i) above (i.e. key study), you have not reported information on the purity of the test material, the distribution of the C-chain length of constituents or the presence of co-solvent (if any). You identified the test material as the Substance but in the endpoint summary record you state that "*in the Key study test solutions of Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium salts (CAS no 85408-62-4) which is a substance very similar to coco fatty acids 2-sulfoethyl sodium salt were prepared*". You indicate that no analytical monitoring of exposure concentrations was conducted. You have not provided an adequate description of the test medium composition including concentrations in DOC, TOC and suspended solids. You have not reported the test concentrations and therefore spacing factor between test concentrations cannot be assessed.

For study (ii) above, you have not reported information on the distribution of the C-chain length of constituents. You report that the free fatty acid content of the test material is 21% while the boundary composition of the substance for Coco fatty acid is < 15%. Therefore the test material does not to the Substance identified in your dossier. You report that an analytical monitoring of exposure was conducted "*using the small scale MBAS method (Methylene Blue Spectraphotometric method)*". You have not reported any performance parameters for the analytical monitoring method including the limit of quantification and a justification that the method allows a specific quantification of the non-hydrolysed form of the test substance.

For study (iii) and (iv) above, you have not reported information on the purity of the test material, the distribution of the C-chain length of constituents or the presence of co-solvent (if any). You indicate that no analytical monitoring of exposure concentrations was conducted.

In your comments on the draft decision you indicate your intention to update the dossier with new data generated for a substance fulfilling the criteria of the SIP and the robust study summaries for these studies. You also indicate that if the new information is not considered sufficient you will perform a new test as per TG 202 on your Substance and change the approach for the information provided on the studies.

Based on the above, none of the studies reported in your technical dossier meets the conditions listed above and therefore these studies do not provide an adequate coverage of the key parameters foreseen to be investigated in an OECD TG 202 study.

Therefore the information requirement is not fulfilled.

3. Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.)

Growth inhibition study aquatic plants is a standard information requirement in Annex VII to REACH.

You have adapted this information requirement according to Annex XI, Section 1.5. of the REACH Regulation and you have provided:

(i) a key study by [redacted] (2008) corresponding to a growth inhibition study to algae and cyanobacteria performed according to OECD TG 201 with SLI (76) stripped with EC no. 287-024-7;
(ii) a supporting study by [redacted] (1985) corresponding to a growth inhibition study to algae and cyanobacteria performed similar to OECD TG 201 with SLI (76) stripped with EC no. 287-024-7.

We have assessed this information and identified the following issues:

A. Tests on substances must be conducted in accordance with the OECD test guidelines or other internationally recognised test method (Article 13(3) of REACH). OECD TG 201 require(s) that the following conditions are met (among others):
   - an adequate description of the test material including purity, the presence (or not) of any co-formulant, the relative abundance of unreacted material(s), the distribution of the c-chain length for the active substance) is provided,
   - the algal biomass in each flask is determined at least daily during the test period and the biomass for each flask at each measuring point must be reported (along with the method for measuring biomass).

   For study (i) above, you have not reported information on the purity of the test material, the distribution of the C-chain length of constituents or the presence of co-solvent (if any). You have provided biomass data at 0h, 48h and 72h. However, you have not provided biomass data at 24h.

   For study (ii) above, you have not reported information on the purity of the test material, the distribution of the C-chain length of constituents or the presence of co-solvent (if any). You report that an analytical monitoring of exposure concentrations was conducted but you have not specified the method used and you have not reported any performance parameters for the analytical monitoring method including the limit of quantification and a justification that the method allows a specific quantification of the non-hydrolysed form of the test substance. You indicate that a vehicle was used but the chemical identity is not specified. You have not provided the algal biomass data in for each flask at each measuring point.

   Based on the above, none of the studies reported in your technical dossier meets the conditions listed above and therefore these studies do not provide an adequate coverage of the key parameters foreseen to be investigated in an OECD TG 201 study.

B. For the reasons detailed in the General considerations section the read-across approach to SLI (76) stripped is rejected.

Therefore the information requirement is not fulfilled.

In your comments on the draft decision you agreed that OECD 201 testing should be carried out with analytical confirmation of dose/exposure concentrations in the media.

4. Ready biodegradability (Annex VII, Section 9.2.1.1.)

Ready biodegradability is a standard information requirement in Annex VII to REACH.

You have provided in your dossier:

(i) a key study by [redacted] (1992) corresponding to ready biodegradability study performed according to OECD TG 301D with the Substance;
(ii) a supporting study by [redacted] (1994) corresponding to ready biodegradability study performed according to OECD TG 301E with the Substance;
(iii) a supporting study by [redacted] (1983) corresponding to ready biodegradability study without specifications on the method used with the Substance;
(iv) a supporting study by [redacted] (1983) corresponding to a ready biodegradability study performed according to OECD TG 301B with the Substance.

We have assessed this information and identified the following issues:

A. Tests on substances must be conducted in accordance with the OECD test guidelines or other internationally recognised test method (Article 13(3) of REACH). OECD TG 301D requires that the following conditions are met (among others):
   - an adequate description of the test material including purity, the presence (or not) of any co-formulant, the relative abundance of unreacted material(s), the distribution of the C-chain length for the active substance) is provided,
   - the calculation of the ThO_2 needs to be provided. If the ThOD cannot be calculated, the COD must be determined,
   - data on the inoculum concentration used to conduct the test need to be provided (in ml effluent/l and in approx. cells/l),
   - adequate information to verify that the validity criteria of the test method were fulfilled, including oxygen depletion in inoculum blank and residual concentrations of oxygen in test bottles,
   - scientific reasons and explanation for any change of procedure from the conditions specified in the technical guideline,
   - O_2 consumption data in tabular form must be provided.

   The key study (see study (i) listed above) was conducted according to OECD TG 301D. You report that the purity of the test material is 82%. You have not reported information on the distribution of the C-chain length of constituents or the presence of co-solvent (if any). You have not reported how the ThOD was calculated nor any information on the COD of the test material. You state that "*the sludge was diluted to a concentration of 2 mg DW/L in the BOD bottles*" but have not reported information on the inoculum concentration in in ml effluent/l and in approx. cells/l. You state that "*the validity of the test is demonstrated by an endogenous respiration of 1.1 mg/L at day 28* [and] *by oxygen concentrations ~0.5 mg/L in the bottles*". You report deviations from the procedure described in the test guideline, including the use of activated sludge as an inoculum instead of a secondary effluent or alternatively surface water, and that ammonium chloride was omitted from the medium to prevent nitrification. You have not provided a justification that these deviations would not impact the validity of the test. You have not provided O_2 consumption data in tabular form measured in blank and test BOD bottles.

   The study (i) does not comply with the conditions listed above and therefore these studies do not provide an adequate coverage of the key parameters foreseen to be investigated in an OECD TG 301D study. In particular, in the absence of information supporting that the bacterial density of the inoculum was within the range specified in OECD TG 301D (10^4-10^6 approx. cells/L) and that the endogeneous respiration in blank bottles was below 1.5 mg/L under the standard conditions soecified in the technical guideline, the use of sewage sludge as an inoculum is not scientifically justified. You

also have not justified that the absence of ammonium chloride in the test medium is an acceptable deviation as it may artificially reduce the measured endogeneous respiration in blank bottles. Finally your robust study summary does not include adequate information for the points listed above. Therefore study (i) is not appropriate to conclude on the ready biodegradability of the Substance

B. Appropriate test guidelines are selected based on the applicability domain of the test guidelines and properties of the substance (ECHA Guidance Chapter R.7b, Section 7.9. and OECD TG 301 and OECD TG 310). For highly adsorptive substances the test guidelines OECD TG 301E is not considered applicable unless an abiotic control is included in the study.

   The study (ii) listed above was conducted according to OECD TG 301E. You have not reported the result of an abiotic control to quantify removal due to adsorption. You report that based on a study conducted according to OECD TG 115 the surface tension of the Substance was determined to be 24 mN/m at 1 g/L (23°C and pH 7) and the substance is ionisable. In section 3.5 of your technical dossier, you report that the substance is used by professionals and consumers in cleaning agents and in cosmetic products with a technical function as surface active agent. Therefore the substance has high adsorption potential.

   Therefore study (ii) is not appropriate to conclude on the ready biodegradability of the Substance.

C. Tests on substances must be conducted in accordance with the OECD test guidelines or other internationally recognised test method (Article 13(3) of REACH). OECD TG 301 specifies that degradation must be followed by the determination of parameters such as DOC, CO2 production and oxygen uptake.

   In study (iii) above, the parameter monitored is the disapperance of the test substance as measured using the Methylene Blue Anionic Surface active spectrophotometry (MBAS). Therefore it does not provide an measure of the mineralization of the test substance.

   Therefore study (iii) is not appropriate to conclude on the ready biodegradability of the Substance.

D. Tests on substances must be conducted in accordance with the OECD test guidelines or other internationally recognised test method (Article 13(3) of REACH). OECD TG 301B requires that the following conditions are met (among others):
   - adequate information need to be provided on the identity of the tests material including purity, the presence (or not) of any co-formulant, the relative abundance of unreacted material(s), the distribution of the C-chain length for the active substance,
   - the calculation of the ThCO2 needs to be provided,
   - data on inorganic carbon (IC) content of the test substance suspension in the mineral medium need to be provided,
   - data on the inoculum concentration used to conduct the test need to be provided (in mg/L SS and in approx. cells/L),
   - the source of the inoculum and any adaptation to the test substance must be described,
   - CO_2 production data in tabular form must be provided.

For study (iv) above, you have not provided a description of the C-chain length distribution of the test material. You have not reported how the ThCO2 was calculated. You have not reported data on inorganic carbon (IC) content of the test substance suspension in the mineral medium. You describe the inoculum as "*sewage microorganisms*" but you have not specified the source of the inoculum and whether or not it was adapted to the test substance. You have not specified the incolcum density at the start of the test period. You have not provided a detailled reporting of the CO_2 production data in tabular form.

Therefore the documentation of this study is insufficient and does not allow an independent assessment of the adequacy of this study, its results and its use for hazard assessment. Hence study (iv) is not appropriate to conclude on the ready biodegradability of the Substance.

In your comments on the draft decision, you indicate your intention to update the robust study summaries for these studies and change if necessary the approach to supporting studies. You also indicate that the test results of the OECD TG 303A will be changed to supporting studies.

Therefore the information requirement is not fulfilled.

Appendix B: Reasons for the requests to comply with Annex VIII of REACH

Under Articles 10(a) and 12(1) of REACH, a technical dossier registered at 10 to 100 tonnes or more per year must contain, as a minimum, the information specified in Annexes VII and VIII to REACH.

1. Screening for reproductive/developmental toxicity (Annex VIII, Section 8.7.1.)

A Screening for reproductive/developmental toxicity study (test method: EU B.63/OECD TG 421 or EU B.64/OECD TG 422) is a standard information requirement in Annex VIII to REACH.

You have adapted this information requirement according to Annex XI, Section 1.5. of the REACH Regulation and you have provided:

(i) a key study by Senn (2008) corresponding to a Screening for reproductive/ developmental toxicity study performed according to OECD TG 421 with the analogue substance Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium salts (SLI (76) stripped; EC no. 287-024-7).

For the reasons detailed in the General considerations section the read-across approach to Milled SLI (76) is rejected.

Based on the above, the information you provided do not fulfil the information requirement.

In your comments on the draft decision you indicate your intention to clarify the identity of the tested substance. You also intend to update and extend the information provided in the document supporting the read-across.

Study design

A study according to the test method EU B.63/OECD TG 421 or EU B.64/OECD TG 422 must be performed in rats with oral (ECHA Guidance R.7a, Section R.7.6.2.3.2.) administration of the Substance.

2. Short-term toxicity testing on fish (Annex VIII, Section 9.1.3.)

Short-term toxicity testing on fish is a standard information requirement in Annex VIII to REACH.

You have provided in your dossier:

(i) a key study by [redacted] (1984) corresponding to a short-term toxicity to fish study performed similar to OECD TG 203 with the Substance;
(ii) a supporting study by [redacted] (1992) corresponding to a short-term toxicity to fish study performed according to OECD TG 203 / EU method C.1 with the Substance;
(iii) a supporting study by [redacted] (1994) corresponding to a short-term toxicity to fish study performed according to OECD TG 203 with the Substance;
(iv) a supporting study by [redacted] (1983) corresponding to a short-term toxicity to fish study performed according to OECD TG 203 with the Substance.

We have assessed this information and identified the following issue:

Tests on substances must be conducted in accordance with the OECD test guidelines or another internationally recognised international test method (Article 13(3) of REACH). OECD TG 203 requires that all the following conditions are met (among others):

- an adequate description of the test material including purity, the presence (or not) of any co-formulant, the relative abundance of unreacted material(s), the distribution of the C-chain length for the active substance) is provided,
- an analytical monitoring of exposure concentrations is provided (including method description and results),
- an adequate description of the test medium is provided (including pH, hardness, Ca/Mg ratio, Na/K ratio, alkalinity, conductivity, DOC and suspended solid content),
- the spacing factor between test concentrations should not exceed 2.2.

For study (i) above, you have not reported information on the distribution of the C-chain length of constituents. You report that the free fatty acid content of the test material is 21% while the boundary composition of the substance for Coco fatty acid is < 15%. Therefore the test material does not fit the Substance Identity Profile (SIP) of the Substance. You report that an analytical monitoring of exposure was conducted "*using the small scale MBAS method (Methylene Blue Spectraphotometric method)*". You have not reported any performance parameters for the analytical monitoring method including the limit of quantification and a justification that the method allows a specific quantification of the non-hydrolysed form of the test substance. You define the test medium as "[redacted] *carbon filtered tap water*" but you have not provided information on the content in particulate matter, TOC and COD.

For study (ii) above, you report that the purity of the test material is 82%. You have not reported information on the distribution of the C-chain length of constituents or the presence of co-solvent (if any). You indicate that no analytical monitoring of exposure concentrations was conducted. You have not provided information on the content in particulate matter, TOC and COD of the test medium.

For study (iii) above, you have not reported information on the distribution of the C-chain length of constituents. You report that the free fatty acid content of the test material is 19 ± 2 % while the boundary composition of the substance for Coco fatty acid is < 15%. Therefore the test material does not fit the Substance Identity Profile (SIP) of the Substance. You indicate that no analytical monitoring of exposure concentrations was conducted. You have not provided information on the content in particulate matter, TOC and COD of the test medium.

For study (iii) above, you have not reported information on the purity and on the C-chain length of constituents of the test material. You indicate that no analytical monitoring of exposure concentrations was conducted. You have not provided information on the content in particulate matter, TOC and COD of the test medium. The spacing factor of test concentrations was above 2.2.

Based on the above none of the studies reported in your technical dossier meets the conditions listed above and therefore these studies do not provide an adequate coverage of the key parameters foreseen to be investigated in an OECD TG 203 study.

In your comments on the draft decision you indicate your intention to update the robust study summaries for these studies. You also indicate that if the new information is not considered sufficient you will change the approach for the information provided on the studies to a Weight of evidence approach.

Therefore the information requirement is not fulfilled.

3. Hydrolysis as a function of pH (Annex VIII, Section 9.2.2.1.)

Hydrolysis as a function of pH is a standard information requirement in Annex VIII to REACH.

You have adapted the information with reference to Annex VIII, Section 9.2.2.1., Column 2.

This information requirement can be adapted according to column 2 of Annex VIII, if the substance is readily biodegradable.

You justified the adaptation by stating that the substance is readily biodegradable. However, the information you provided for Ready biodegradability (Annex VII, Section 9.2.1.1.) cannot be considered to be reliable as explained under request A.4 above. Therefore, it cannot be used to waive the endpoint Hydrolysis as a function of pH.

In your comments on the draft decision you indicate your intention to update the robust study summary for the ready biodegradability study.

Therefore the information requirement is not fulfilled.

4. Adsorption/desorption screening (Annex VIII, Section 9.3.1.)

Adsorption/desorption screening is a standard information requirement in Annex VIII to REACH.

You have adapted this information requirement according to Annex XI, Section 1.5. of the REACH Regulation and you have provided:

(i) a key study by [redacted] (2009) corresponding to an adsorption / desorption: screening study performed according to OECD TG 106 with the source substance Dodecanoic acid, 2-sulfoethyl ester, sodium salt (EC no. 230-949-8 / CAS no. 7381-01-3).

We have assessed this information and identified the following issues:

A. Tests on substances must be conducted in accordance with the OECD test guidelines or other internationally recognised test method (Article 13(3) of REACH). OECD TG 106 aims at estimating the adsorption/desorption behaviour of a substance in soils.

   You have provided a single study by [redacted] (2009) performed according to OECD TG 106 with radiolabelled Dodecanoic acid, 2-sulfoethyl ester, sodium salt (SLI) performed on sewage sludge. Your report that the log Koc of the test material was 3.2.

   The study reported in your technical dossier was conducted on sewage sludge and not on soils and therefore it does not provide an adequate coverage of the key parameter foreseen to be investigated in an OECD TG 106 study.

B. For the reasons detailed in the General considerations section the read-across approach to Dodecanoic acid, 2-sulfoethyl ester, sodium salt (SLI) is rejected.

In your comments on the draft decision you indicate your intention to provide new information for this information requirement based on existing studies for another substance. You indicate in case this new information is not considered as sufficient that you will perform a new test.

Therefore the information requirement is not fulfilled.

Appendix C: Reasons for the requests to comply with Annex IX of REACH

Under Articles 10(a) and 12(1) of REACH, a technical dossier registered at 100 to 1000 tonnes or more per year must contain, as a minimum, the information specified in Annexes VII to IX to REACH.

1. Sub-chronic toxicity study (90-day), oral route (Annex IX, Section 8.6.2.)

A Sub-chronic toxicity study (90 day) is a standard information requirement in Annex IX to REACH.

You have adapted this information requirement according to Annex XI, Section 1.5. of the REACH Regulation and you have provided:

(i) a key study by [redacted] (2009) corresponding to a sub-chronic toxicity study (90 day) performed according to OECD TG 408 with the source substance sodium 2-hydroxyethanesulfonate (EC no. 216-343-6).

For the reasons detailed in the General considerations section the read-across approach to sodium 2-hydroxyethanesulfonate is rejected.

Therefore the information requirement is not fulfilled.

In your comments on the draft decision you indicate your intention to strenghten the read-across argumentation and to update the dossier with the new justification.

Study design

Referring to the criteria provided in Annex IX, Section 8.6.2, Column 2, the oral route is the most appropriate route of administration to investigate repeated dose toxicity, because the Substance is a solid and is marketed or supplied in a mixture as cleaning agents and in cosmetic and personal care products.

Therefore the sub-chronic toxicity study must be performed according to the OECD TG 408, in rats and with oral administration of the Substance

2. Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.) in a first species

A Pre-natal developmental toxicity (PNDT) study (OECD TG 414) in one species is a standard information requirement under Annex IX to REACH.

You have adapted this information requirement according to Annex XI, Section 1.5. of the REACH Regulation and you have provided:

(i) a key study by [redacted] (2008) corresponding to a Pre-natal developmental toxicity (PNDT) study performed according to OECD TG 414 with the analogue substance Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium salts (Milled SLI (76); EC no. 287-024-7).

For the reasons detailed in the General considerations section the read-across approach to Milled SLI (76) is rejected.

Based on the above, the information you provided do not fulfil the information requirement.

In your comments on the draft decision you indicate your intention to clarify the identity of the tested substance. You also intend to update and extend the information provided in the document supporting the read-across.

Study design

A PNDT study according to the test method OECD TG 414 must be performed in rat or rabbit as preferred species with oral (ECHA Guidance R.7a, Section R.7.6.2.3.2.) administration of the Substance.

3. Long-term toxicity testing on aquatic invertebrates (Annex IX, Section 9.1.5.) and

4. Long-term toxicity testing on fish (Annex IX, Section 9.1.6.1.)

Long-term toxicity testing on aquatic invertebrates and fish are standard information requirements in Annex IX to the REACH Regulation.

You have adapted these information requirements according to Annex IX, Section 9.1., Column 2. For long-term toxicity on aquatic invertebrates you have provided the following justification: "*According to Annex IX, 9.1.5 to the REACH Regulation long-term toxicity testing with daphnia shall be proposed if the CSA indicates the need to investigate further the effects on aquatic organisms. However, as the CSA does not indicate the need for further testing of invertebrates and taking into consideration the low bioaccumulation potential, long-term toxicity testing with daphnia is waived*". For long-term toxicity on fish you have provided the following justification: "*According to Annex IX, 9.1.6 to the REACH Regulation long-term toxicity testing with fish shall be proposed only if the CSA indicates the need to investigate further the effects on aquatic organisms. However, as the CSA does not indicate the need for further testing of vertebrates and taking into consideration the low bioaccumulation potential, long-term toxicity testing with fish is waived*".

We have assessed this information and identified the following issue:

As specified in Annex IX, Section 9.1., Column 2, a long-term toxicity to study on aquatic invertebrates and/or on fish must be performed unless the Chemical Safety Assessment demonstrates that risks towards the aquatic compartment arising from the use of the Substance are controlled (as per Annex I, section 0.1). The justification must be documented in the Chemical Safety Assessment.

In particular, the Chemical Safety Assessment must take into account the following elements to support that long-term toxicity testing is not required:

- all relevant hazard information from your registration dossier,
- the outcome of the exposure assessment in relation to the uses of the Substance,
- the outcome of the PBT/vPvB assessment including information on relevant degradation products and constituents present in concentration at or above 0.1% (w/w).

You did not submit in your dossier any specific justification as to why the risks of the substance are controlled. However, to reach the conclusion that the risks are controlled, we understand that you rely on the results of acute aquatic toxicity data included in your dossier (used for PNEC derivation) and the outcome of the exposure assessment showing risk characterisation ratios (RCRs) below 1 for the freshwater and marine aquatic compartments.

As specified in request A.2, A.3 and B.2, the data on short-term toxicity to aquatic invertebrates and fish and on growth inhibition to algae and cyanobacteria are not compliant. Hence your dossier currently does not include adequate information to characterize the hazard property of the Substance.

Without this information your Chemical Safety Assessment does not demonstrate that the risks of the Substance are adequately controlled.

Therefore, your adaptations according to Annex IX, Section 9.1., Column 2 are rejected and the information requirements for long-term toxicity on aquatic invertebrates and on fish are not fulfilled.

In your comments on the draft decision you indicate your intention to provide a robust justification in accordance with Column 2 of Annex IX section 9.1 demonstrating that risks towards the aquatic compartment following exposure to the registration substance are adequately controlled and/or to include any available relevant data on long term toxicity to aquatic invertebrates and fish.

5. **Simulation testing on ultimate degradation in surface water (Annex IX, Section 9.2.1.2.)**

   and

6. **Sediment simulation testing (Annex IX, Section 9.2.1.4.)**

Simulation testing on ultimate degradation in surface water is a standard information requirement in Annex IX to REACH.

Sediment simulation testing is a standard information requirement in Annex IX to REACH for substances with a high potential for adsorption to sediment. The Substance has low surface tension 24 mN/m at 1 g/L (23°C and pH 7), is used in various consumer and professional products with a technical function as surface active agent and is ionisable, indicating high adsorptive properties. Therefore the sediment compartment is relevant to evaluate the fate of the Substance.

You have adapted these information requirements by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. and you have provided in your dossier a key study by [redacted] (2010) corresponding to simulation test – Activated sludge unit according to OECD TG 303A with radiolabelled ^{14}C Sodium Lauryl Isethionate.

You have also adapted these information requirements based on Annex IX, Section 9.1.1.2. and Section 9.2.1.4., Column 2 with the following justification: "*the study does not need to be conducted because the substance is readily biodegradable*".

We have assessed this information and identified the following issues:

A. For the reasons detailed in the General considerations section the read-across approach to SLI is rejected.

B. The information used for the purpose of assessment of the PBT/vPvB properties must be based on data obtained under relevant conditions (Annex XIII). The test conducted

must simulate degradation in a relevant environment i.e. regarded as equivalent to a simulation test in surface water or in sediment (ECHA Guidance R.11.4).

The study by [redacted] (2010) according to OECD TG 303A is a test to simulate degradation in an aerobic sewage treatment plant. The study by [redacted] (2010) according to OECD TG 3014D is a test to simulate biodegradation in treated effluent-surface water mixing zone. None of these studies are regarded as equivalent to a simulation test in relevant environment such as fresh or estuarine water, marine water or fresh or estuarine sediment or marine sediment.

C. Simulation testing on ultimate degradation in surface water does not need to be conducted if the substance is highly insoluble in water or is readily biodegradable (Annex IX, Section 9.2.1.2, Column 2). Sediment simulation testing does not need to be conducted if the substance is readily biodegradable or direct and indirect exposure of sediment is unlikely (Annex IX, Section 9.2.1.4, Column 2).

As explained under request A.4 you have not provided reliable information to conclude that the Substance is readily biodegradable. Furthermore the absence of exposure of the aquatic and sediment compartments has not been demonstrated:

- based on the reported uses, sediment exposure cannot be excluded. You report wide dispersive professional and consumer uses with Environmental Release Category (ERC) 8a and also that the exposure estimations that you provided in the Chemical Safety Report (CSR) indicate that there is exposure to water and sediment in number of your exposure scenarios.
- you report that that based on a study conducted according to OECD TG 115 the critical micelle concentration of the substance is 102 mg/L (23°C and pH 7). Therefore the Substance is not highly insoluble.
- you report that based on a study conducted according to OECD TG 115 the surface tension of the Substance was determined to be 24 mN/m at 1 g/L (23°C and pH 7) and the substance is ionisable. In section 3.5 of your technical dossier, you report that the substance is used by professionals and consumers in cleaning agents and in cosmetic products with a technical function as surface active agent. Therefore the substance has high adsorption potential.

Hence your adaptation according to Annex IX, Section 9.2.1.2. and 9.2.1.4, Column 2 are rejected.

Therefore the information requirements are not fulfilled.

In your comments on the draft decision you indicate your intention to update the robust study summary for the ready biodegradability study and to use this information to waive the requirement for simulation testing on ultimate degradation in surface water and sediment in accordance with REACH Annex IX, Sections 9.2.1.2. and 9.2.1.4., Column 2, respectively.

Study design

Under Annex XIII, the information must be based on data obtained under conditions relevant for the PBT/vPvB assessment. Therefore:

- You must perform the OECD TG 309 test, by following the pelagic test option with natural surface water containing approximately 15 mg dw/L of suspended solids (acceptable concentration between 10 and 20 mg dw/L) (ECHA Guidance R.11).

- You must perform the test at the temperature of 12 °C, the average environmental

temperature for the EU (ECHA Guidance R.16, Table R.16-8). Performing the tests at this temperature is in line with the applicable test conditions of the OECD TG 308 and TG 309.

Non-extractable residues (NER) must be quantified in all simulation studies. The reporting of results must include a scientific justification of the used extraction procedures and solvents. By default, total NER is regarded as non-degraded Substance. However, if reasonably justified and analytically demonstrated a certain part of NER may be differentiated and quantified as irreversibly bound or as degraded to biogenic NER. Such fractions could be regarded as removed when calculating the degradation half-life(s) (ECHA Guidance Chapter R.11).

7. Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.), aqueous exposure

Bioaccumulation in aquatic species, preferably fish is a standard information requirement in Annex IX to REACH.

You have adapted this information requirement Annex IX, Section 9.3.2., Column 2 with the following justification: "*the study does not need to be conducted because the substance has a low potential for bioaccumulation based on log Kow <= 3*".

We have assessed this information and identified the following issue:

Annex IX, Section 9.3.2., column 2 specifies that a study does not need to be conducted if the substance has a low potential for bioaccumulation (for instance a log Kow ≤ 3). To adapt this information requirement based on low potential to partition to lipids (i.e. log Kow ≤ 3), lipophilicity must be the sole characteristic driving the bioaccumulation potential of a substance. However, for some groups of substances (e.g. organometals, ionisable substances, surfactants) other mechanisms than partitioning to lipids may drive bioaccumulation (e.g. binding to protein/cell membranes). For those substances log Kow is not considered a valid descriptor of the bioaccumulation potential and therefore for measured BCF values are preferred (ECHA Guidance R.7c, Appendix R.7.10-3).

You have justified the low potential low potential for bioaccumulation because the partition coefficient value (log Kow) was determined to be -0.41 based on the ratio of the octanol solubility and the CMC of the Substance.

The Substance is surface active (with a surface tension in water of 24 mN/m at 1 g/L and 23°C) and is ionisable. Hence binding to protein/cell membranes cannot be excluded. Therefore log Kow is not a valid descriptor for assessing the bioaccumulation potential of the Substance and your adaptation is rejected.

Therefore, the information requirement is not fulfilled.

In your comments on the draft decision you indicate your intention to investigate whether a weight-of-evidence (WoE) approach could demonstrate a lack of bioaccumulation potential.

Study design

Bioaccumulation in fish: aqueous and dietary exposure (test method EU C.13. / OECD TG 305) is the preferred test to investigate bioaccumulation (ECHA Guidance R.7c, Section R.7.10.3.1). Whenever technically feasible, the aqueous route of exposure (OECD TG 305-I)

must be used as the results obtained can be used directly for comparison with the B and vB criteria of Annex XIII of REACH. Therefore, the requested study must be conducted with aqueous exposure. If testing through aquatic exposure is technically not possible, you must provide scientifically valid justification for the infeasibility.

Appendix D: Procedural history

For the purpose of the decision-making, this decision does not take into account any updates of registration dossiers after the date on which you were notified the draft decision according to Article 50(1) of REACH.

The compliance check was initiated on 12 April 2019.

The decision making followed the procedure of Articles 50 and 51 of the REACH Regulation, as described below:

ECHA notified you of the draft decision and invited you to provide comments within 30 days of the notification.

ECHA took into account your comments did not amend the requests.

ECHA notified the draft decision to the competent authorities of the Member States for proposals for amendment.

As no amendments were proposed, ECHA adopted the decision under Article 51(3) of REACH.

Appendix E: Observations and technical guidance

1. This compliance check decision does not prevent ECHA from initiating further compliance checks at a later stage on the registrations present.

2. Failure to comply with the requests in this decision, or to otherwise fulfil the information requirements with a valid and documented adaptation, will result in a notification to the enforcement authorities of the Member States.

3. Test guidelines, GLP requirements and reporting

   Under Article 13(3) of REACH, all new data generated as a result of this decision needs to be conducted according to the test methods laid down in a European Commission Regulation or according to international test methods recognised by the Commission or ECHA as being appropriate.

   Under Article 13(4) of REACH, ecotoxicological and toxicological tests and analyses shall be carried out according to the GLP principles (Directive 2004/10/EC) or other international standards recognised by the Commission or ECHA.

   Under Article 10 (a) (vi) and (vii) of REACH, all new data generated as a result of this decision must be reported as study summaries, or as robust study summaries, if required under Annex I of REACH. See ECHA Practical Guide: 'How to report robust study summaries'[6].

4. Test material

   Selection of the test material(s)

   The registrants of the Substance are responsible for agreeing on the composition of the test material to be selected for carrying out the tests required by the present decision. The test material selected must be relevant for all the registrants of the Substance, i.e. it takes into account the variation in compositions reported by all members of the joint submission. The composition of the test material(s) must fall within the boundary composition(s) of the Substance.

   While selecting the test material you must take into account the impact of each constituent/ impurity on the test results for the endpoint to be assessed. For example, if a constituent/ impurity of the Substance is known to have an impact on (eco)toxicity, the selected test material must contain that constituent/ impurity.

   Technical reporting of the test material

   The composition of the selected test material must be reported in the respective endpoint study record, under the Test material section. The composition must include all constituents of the test material and their concentration values. Without such detailed reporting, ECHA may not be able to confirm that the test material is relevant for the Substance and to all the registrants of the Substance.

   Technical instructions are available in the manual "How to prepare registration and PPORD dossiers"[7].

[6] https://echa.europa.eu/practical-guides
[7] https://echa.europa.eu/manuals

5. Strategy for the PBT/vPvB assessment

You are advised to consult ECHA Guidance R.7b, Section R.7.9., R.7c, Section R.7.10 and R.11 on PBT assessment to determine the sequence of the tests and the necessity to conduct all of them. The guidance provides advice on 1) integrated testing strategies (ITS) for the P, B and T assessments and 2) the interpretation of results in concluding whether the Substance fulfils the PBT/vPvB criteria of Annex XIII.

You are advised to first conclude whether the Substance may fulfil the Annex XIII criteria of being P or vP, and then continue with the assessment for bioaccumulation. The sequence of the simulation tests also needs to consider the intrinsic properties of the Substance, its identified use and release patterns as these could significantly influence the environmental fate of the Substance. You shall revise the PBT assessment when the new information is available.

6. List of references of the ECHA Guidance and other guidance/ reference documents[8]

Evaluation of available information
Guidance on information requirements and chemical safety assessment, Chapter R.4 (version 1.1., December 2011), referred to as ECHA Guidance R.4 in this decision.

QSARs, read-across and grouping
Guidance on information requirements and chemical safety assessment, Chapter R.6 (version 1.0, May 2008), referred to as ECHA Guidance R.6 in this decision.

ECHA Read-across assessment framework (RAAF, March 2017)[9]

Physical-chemical properties
Guidance on information requirements and chemical safety assessment, Chapter R.7a (version 6.0, July 2017), referred to as ECHA Guidance R.7a in this decision.

Toxicology
Guidance on information requirements and chemical safety assessment, Chapter R.7a (version 6.0, July 2017), referred to as ECHA Guidance R.7a in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.7c (version 3.0, June 2017), referred to as ECHA Guidance R.7c in this decision.

Environmental toxicology and fate
Guidance on information requirements and chemical safety assessment, Chapter R.7a (version 6.0, July 2017), referred to as ECHA Guidance R.7a in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.7b (version 4.0, June 2017), referred to as ECHA Guidance R.7b in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.7c (version 3.0, June 2017), referred to as ECHA Guidance R.7c in this decision.

PBT assessment

[8] https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment
[9] https://echa.europa.eu/support/registration/how-to-avoid-unnecessary-testing-on-animals/grouping-of-substances-and-read-across

Guidance on information requirements and chemical safety assessment, Chapter R.11 (version 3.0, June 2017), referred to as ECHA Guidance R.11 in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.16 (version 3.0, February 2016), referred to as ECHA Guidance R.16 in this decision.

OECD Guidance documents[10]
Guidance Document on aqueous–phase aquatic toxicity testing of difficult test chemicals – No 23, referred to as OECD GD23.
Guidance Document on Mammalian Reproductive Toxicity Testing and Assessment – No 43, referred to as OECD GD43.

[10] http://www.oecd.org/chemicalsafety/testing/series-testing-assessment-publications-number.htm

Appendix F: List of the registrants to which the decision is addressed and the corresponding information requirements applicable to them

Registrant Name	Registration number	(Highest) Data requirements to be fufilled
[redacted]	[redacted]	[redacted]

Note: where applicable, the name of a third party representative (TPR) may be displayed in the list of recipients whereas the decision is sent to the actual registrant.