EUROPEAN CHEMICALS AGENCY

Helsinki, 27 May 2020

Addressee
Registrant of JS_156572-81-5 listed in the last Appendix of this decision

Date of submission for the jointly submitted dossier subject of this decision
22/02/2018

Registered substance subject to this decision, hereafter 'the Substance'
Substance name: sodium 2-(dodecanoyloxy)propane-1-sulfonate
EC number: 700-150-3
CAS number: 156572-81-5

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 September 2023***.

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

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

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

3. 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. In vitro cytogenicity study in mammalian cells (Annex VIII, Section 8.4.2., test method: OECD TG 473) or in vitro micronucleus study (Annex VIII, Section 8.4.2., test method: OECD TG 487) with the Substance

2. Only if a negative result in Annex VIII, Section 8.4.2. is obtained, In vitro gene mutation study in mammalian cells (Annex VIII, Section 8.4.3.; test method: OECD TG 476 or TG 490) with the Substance

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

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

5. 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

D. Requirements applicable to all the Registrants subject to Annex X of REACH

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

2. Long-term toxicity to sediment organisms (Annex X, Section 9.5.1.; test design: OECD TG 218 or OECD TG 225 or OECD TG 233) with the Substance

Conditions to comply with the requests

You are bound by the requests for information corresponding to the REACH Annexes applicable to your own registered tonnage of the Substance at the time of evaluation.

Therefore you have to comply with the requirements of Annexes VII to X of REACH as you have registered the Substance at above 1000 tpa.

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.3 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 standard information requirements listed below by applying read-across approaches in accordance with Annex XI, Section 1.5:

- In vitro cytogenicity study in mammalian cells or in vitro micronucleus study (Annex VIII, Section 8.4.2.)
- In vitro gene mutation study in mammalian cells (Annex VIII, Section 8.4.3.)
- Short-term repeated dose toxicity (28 day), (Annex VIII, Section 8.6.1.)
- Sub-chronic toxicity study (90-day), (Annex IX, Section 8.6.2.)
- Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.)
- Ready biodegradability (Annex VII, Section 9.2.1.1.)
- Simulation testing on ultimate degradation in surface water (Annex VIII, Section 9.2.)
- Short-term toxicity testing on aquatic invertebrates (Annex VII, Section 9.1.1.)
- Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.)
- Short-term toxicity testing on fish (Annex VIII, Section 9.1.3.)

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 (addressed under 'Assessment of prediction(s)').

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

A. Predictions for toxicological properties

You have provided the following reasoning for the prediction of toxicological properties: "*The target (SLMI) and four source substances have very similar structures and sizes, and the available physico-chemical data of all five substances are comparable (varying only as would be expected to account for different fatty acid chain lengths). All would be expected to undergo the same, rapid biotransformations in vivo. Metabolism would be expected to result in straight chain fatty acids (C8 to C18, innocuous components of the mammalian diet) and either sodium isethionate (SCI/SLI) or sodium methylisethionate (SLMI/SCMI/SDMI).*
There are no functional groups novel to the target substance, and no structural alerts in the target or source compounds that are indicative of mutagenicity, carcinogenicity or skin sensitisation. Indeed, where available, the existing dataset on the five substances consistently indicate that this closely-related group is of low acute and repeated dose toxicity, and there is no evidence of skin sensitisation, genotoxic and carcinogenic activity, or of reproductive and developmental toxicity. Overall, SLMI and the four source substances are all considered

of low concern for human health. However, there is evidence that SLMI, SCI and SCMI are mild-to-moderate skin irritants and SCI is an eye irritant".

ECHA understands that you predict the toxicological properties of the Substance using a read-across hypothesis which assumes that different compounds have the same type of effects.

The toxicological properties of the Substance are predicted to be quantitatively equal to those of the source substances. Furthermore, you argue that the target and the source substances have similar bio-transformation products.

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

1. Fatty acids, coco, 2-sulfoethyl esters, sodium salts (SCI) with EC no. 263-052-5 which is used a source substance for:
   - In vitro cytogenicity study in mammalian cells or in vitro micronucleus study (Annex VIII, Section 8.4.2.); [redacted] (1991) and [redacted] (2008)
   - In vitro gene mutation study in mammalian cells (Annex VIII, Section 8.4.3.); [redacted] (2007)
   - Short-term repeated dose toxicity (28 day), (Annex VIII, Section 8.6.1.); [redacted] (1995) and [redacted] (1991)

2. [redacted] with no EC or CAS number identified is referred as a source substance for Sub-chronic toxicity study (90-day) (Annex IX, Section 8.6.2.) in your read across justification (and in a data matrix) but no study with this substance is included in the dossier.

3. Sodium 2-sulphonatoethyl laurate (SLI) with EC no. 230-949-8 for toxicokinetics ([redacted] 1974; 1975 and [redacted] 2010)

4. Coco fatty acids 1-methyl-2-sulfoethyl ester, sodium salt /Sodium cocoyl methyl isethionate (SCMI) with CAS no. 869861-16-5 which is not used for any toxicological endpoints.

Sodium isethionate (SI) with EC no. 216-343-6 is not referred as a source substance in your read across justification but a study performed with SI ([redacted] 2009) is included in the technical dossier for the Sub-chronic toxicity study (90-day), (Annex IX, Section 8.6.2.). The shortcomings relating to this read across justification is addressed in the justification for this information requirement.

Fatty acids, C12-18 and C18-unstad., 2-sulfoethyl esters, sodium salts, with CAS no. 85408-62-4 and EC no. 287-024-7 is also not referred to as a source substance in your read across justification but a study performed with this substance ([redacted], 2008) is included in the technical dossier for the, Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.). The shortcomings relating to this read across justification is addressed in the justification for this information requirement.

Concerning the predictions of toxicological properties based on the source substances identified under points 1 to 4 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) must be provided to allow assessment whether the attempted predictions are compromised by the composition and/or impurities.

In your read-across justification document you state that SCI cannot be chemically characterised *"due to the variable composition of "coco fatty acids""*. You provide a generic description of the C-chain distribution of the cocoyl group used in the studies conducted with SCI. In your technical dossier the test materials are described as [redacted] (purity: [redacted]%) or [redacted] (purity: [redacted]%). You have not provided quantitative information on the composition of these test materials including the presence of unreacted starting material and distribution of C-chain length. In addition, concerning the studies conducted on SLI, the test material is described as [redacted] and no information on purity or composition is provided.

In the absense of adequate information on the purity and composition of the test materials used in the studies on the source substances, no qualitative or quantitative comparative assessment of the compositions of the target and source materials 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 substances.

2) Read-across hypothesis contradicted by existing data

As indicated above, your read-across hypothesis is also based on the similar, rapid (bio)transformation of the Substance and of the source substances to a common compound. In this context, information characterising the rate and extent of the hydrolysis of the Substance and of the source substances needs to confirm the similar 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 the Substance and source substances (SCI, SLI and [redacted]) 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 either sodium isethionate (for SCI/SLI) or sodium methylisethionate (for the Substance and SDMI).

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

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

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 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.

3) 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 cause the same type of effect(s). In this context, relevant, reliable and adequate information allowing to compare the properties of the Substance and of the source substance(s) is necessary to confirm that both substances cause the same type of effects. Such information can be obtained, for example, from bridging studies of comparable design and duration for the Substance and of the source substance(s).

However, your dossier does not contain any toxicology data on the Substance for any endpoint except an inconclusive eye irritation study and an Ames study.

Therefore, a direct comparison of the toxicological potency of the Substance and source substances for the endpoints under consideration is not possible. In the absence of such information, you cannot establish that the Substance and the source substances are likely to have similar properties. Consequently, you have not provided sufficient supporting information to strengthen the rationale for the read-across.

4) *Omission 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 be included in the dossier in order to be assessed and to support the read-across justification. In addition they should:

- be adequate for the purpose of classification and labelling and/or risk assessment;
- have adequate and reliable coverage of the key parameters addressed in the corresponding test method referred to in Article 13(3);
  - cover an exposure duration comparable to or longer than the corresponding test method referred to in Article 13(3) if exposure duration is a relevant parameter.

However, some of the source studies that you refer to in your read-across justification document are not included in the IUCLID dossier, more specifically the short-term (Zhejiang, 2013b) and sub-chronic (Zhejiang, 2013c) toxicity studies with the analogue substance SDMI.

Therefore, the omission of this information from the dossier does not allow ECHA to assess and conclude on the relevance of this information regarding the read-across.

B. Predictions for ecotoxicological properties

i. Aquatic toxicity

You have provided the following reasoning for the prediction of aquatic toxicity: "*The available ecotoxicity information on SLMI and SCI includes short-term studies on Daphnia, algae and fish. These indicate that both compounds are harmful to aquatic life. Higher toxicity values*

were reported in equivalent studies of SCMI, suggesting that this analogue is of lower concern for aquatic life".

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 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:

1. Coco fatty acids 1-methyl-2-sulfoethyl ester, sodium salt / Sodium cocoyl methyl isethionate (SCMI) with CAS no. 869861-16-5, which is used as a source substance for:
   - Short-term toxicity testing on aquatic invertebrates (Annex VII, Section 9.1.1.); [redacted] (2005)
   - Short-term toxicity testing on fish (Annex VIII, Section 9.1.3.); [redacted] (2005)
   - Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.); [redacted] (2005)

2. Fatty acids, coco, 2-sulfoethyl esters, sodium salts (SCI) with EC no. 263-052-5, which is used as a source substance for:
   - Short-term toxicity testing on aquatic invertebrates (Annex VII, Section 9.1.1.); [redacted] (1984)
   - Short-term toxicity testing on fish (Annex VIII, Section 9.1.3.); [redacted] (2003)

ECHA notes the following shortcomings with regards to prediction(s) of aquatic toxicity:

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).

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

- [redacted] (2005) used to cover the requirement for a short-term toxicity study to fish;
- [redacted] (1984) used to cover the requirement for a short-term toxicity study to fish;
- [redacted] (2005) used to cover the requirement for a short-term toxicity study to aquatic invertebrates;
- [redacted] (2003) used to cover the requirement for a short-term toxicity to study aquatic invertebrates;
- [redacted] (2005) used to cover the requirement for a toxicity to aquatic 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 where each study is relied upon.

2) Missing supporting information to substantiate worst-case consideration

As indicated above, 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 of

the Substance. In this context, relevant, reliable and adequate information allowing to compare the properties of the Substance and of the source substance(s) is necessary to confirm a conservative prediction of the properties of the Substance from the data on the source substance(s). 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:

- short-term toxicity study on aquatic invertebrates for SCMI, SCI and the Substance,
- short-term toxicity study on fish for SCMI and SCI,
- toxicity studies to aquatic algae and cyanobacteria for SCMI and the Substance.

You consider that information supports that SCMI has higher toxicity than SCI and that it can be used to cover the information requirement for the Substance. You have not discussed differences in effects observed in studies conducted with the Substance and the selected analogue substances.

However, as already explained under issue 1) above, you have not provided any reliable studies on the selected source substances. In addition, as explained further below under the information requirement where each study is relied upon, the studies conducted with the Substance are not reliable. 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.

In the absence of such information, you have not established that the source substance SCMI constitutes a worst-case for the prediction of the property under consideration of the Substance. Therefore you have not provided sufficient supporting information to strengthen the rationale for the read-across.

ii. Biodegradation

You have provided the following reasoning for the prediction of biodegradation: *"SLMI and all of the source compounds are considered "readily biodegradable""*.

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 following source substance Coco fatty acids 1-methyl-2-sulfoethyl ester, sodium salt / Sodium cocoyl methyl isethionate (SCMI) with CAS no. 869861-16-5, which is used as a source substance for Ready biodegradability (Annex VII, Section 9.2.1.1.); [redacted] (2007).
ECHA notes the following shortcomings with regards to prediction(s) of biodegradation:

1) Adequacy and reliability of the 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).

However, the study by [redacted] (2007) 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 where the study is relied upon.

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 ready biodegradability studies on SCMI and the Substance. You consider that these studies support that both substances are readily biodegradable.

However, as already explained under issue 1) above, you have not provided any reliable studies on the selected source substance. In addition, as explained further below under the information requirement for ready biodegradability, the study conducted with the Substance is not reliable. 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 established that relevant properties of the Substance can be predicted from data on the analogue substances. Therefore, your adaptation does not comply with the general rules of adaptation as set out in Annex XI, Section 1.5. and your read-across approach is rejected.

In your comments on the draft decision you consider that it is possible to significantly improve the read-across justification and documentation. You also state that new data may be generated on the substance and/or source substances to either add weight to the read across hypothesis (bridging studies) or address outstanding issues with existing study designs or reporting. Finally you note that in some cases, additional data from studies not requested (including New Approach Methods (NAMs)) may be provided if they add to the WoE for a particular endpoint.

ECHA acknowledges your intention to improve the read across justification and documentation taking into account the issues raised in the decision. You are encouraged to make use of ECHA's Read–Across Assessment Framework (RAAF, March 2017)[7] to check the robustness of your updated read-across adaptation.

(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 the long-term studies on both invertebrates and 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. 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] (2013) corresponding to a short-term toxicity study to aquatic invertebrates performed according to OECD TG 202 with the Substance

You have also adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. and you have provided:

(ii) a supporting study by [redacted] (2005) corresponding to a short-term toxicity study to aquatic invertebrates performed according to EPA OPPTS 850.1010 with the source substance SCMI (CAS no. 869861-16-5)
(iii) a supporting study by [redacted] (2003) corresponding to a short-term toxicity to study aquatic invertebrates performed according to OECD TG 202 with the source substance SCI (EC no. 263-052-5)

We have assessed this information and identified the following issues:

A. Tests on substances must be conducted in accordance with the applicable OECD test guidelines or other internationally recognised test methods (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),
   - the test is conducted on young daphnids (neonates aged less than 24 hours at the start of the test),
   - a description of methods of preparation of stock and test solutions including the use of any solvent or dispersants, concentrations used,
   - 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,
   - the number and percentage of daphnids that were immobilised or showed any adverse effects (including abnormal behaviour) in the controls and in each treatment group is reported.

   For study (i) above, you have not reported information on the purity of the test material or the presence of co-solvent (if any). You report that an analytical monitoring of exposure concentrations was conducted and you state that *"the recovery rates ranged from 97.3% to 120.0%.* [...] *SLMI was stable during the test course"*. You have

not provided a description of the analytical method used and of the results. You have not reported the life-stage of the test organisms. You report that a vehicle was used but you did not describe the chemical identity of the vehicle and how the test solutions were prepared. You have reported some limited information on pH and dissolved oxygen content of the test medium but you have not provided a description of the composition of the dilution water. You have not reported the result of the study (number and percentage of daphnids that were immobilised) for all test conditions in a tabulated form.
For study (ii) above, you have not reported information on the purity of the test material or the presence of co-solvent (if any) and on the distribution of the C-chain length. You specify that no analytical monitoring of exposure concentrations was conducted. You have reported some limited information on pH and dissolved oxygen content of the test medium but you have not provided a description of the composition of the dilution water. You report that the spacing factor between exposure concentrations was 10. You have not reported the result of the study (number and percentage of daphnids that were immobilised) for all test conditions in a tabulated form.
For study (iii) above, you have not reported information on the purity of the test material or the presence of co-solvent (if any) and on the distribution of the C-chain length. You have not reported the life-stage of the test organisms. You specify that no analytical monitoring of exposure concentrations was conducted. You have reported some limited information on pH, hardness and dissolved oxygen content of the test medium but you have not provided a description of the composition of the dilution water.

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.

In your comments on the draft decision you indicate your intention to update the robust study summaries for these studies.

B. For the reasons detailed in the General considerations section the read-across approach to SCMI and SCI is rejected.

Therefore the information requirement is not fulfiled.

2. 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 provided in your dossier:

(i) a key study by [redacted] (2013) corresponding to a growth inhibition study to algae performed according to OECD TG 201 with the Substance

You have also adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. and you have provided:

(ii) a supporting study by [redacted] (2005) corresponding to a growth inhibition study to algae performed according to EPA OPPTS 850.5400 with the source substance SCMI

(CAS no. 869861-16-5)

We have assessed this information and identified the following issues:

A. Tests on substances must be conducted in accordance with the applicable OECD test guidelines or other internationally recognised test methods (Article 13(3) of REACH). OECD TG 201 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),
   - the composition of the test medium and the preparation of test solutions is reported,
   - the spacing factor between test concentrations must not exceed 3.2,
   - the test endpoint is inhibition of growth, expressed as the logarithmic increase in biomass (average specific growth rate) during the exposure period. Yield is only considered an additional parameter,
   - biomass for each flask at each measuring point and method for measuring biomass is reported.

   For study (i) above, you have not reported information on the purity of the test material or the presence of co-solvent (if any). You report that an analytical monitoring of exposure concentrations was conducted and your state that "[the] *recovery rate was determined between 97.3% and 101.7%*". You have not provided a description of the analytical method used and of the results. You have not reported any information on the test medium composition. You have not provided a reporting of the study results (i.e. biomass for each flask at each measuring point) in a tabulated form.

   For study (ii) above, you have not reported information on the purity of the test material or the presence of co-solvent (if any) and on the distribution of the C-chain length. You specify that no analytical monitoring of exposure concentrations was conducted. You report that the spacing factor between exposure concentrations was 10. You report effect value in cell number and you have not provided any information on growth rate. You have not provided a reporting of the study results (i.e. biomass for each flask at each measuring point) in a tabulated form.

   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.

   In your comments on the draft decision you indicate your intention to update the robust study summaries for these studies.

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

Therefore the information requirement is not fulfiled.

3. 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] (2012) corresponding to a ready biodegradability test performed according to OECD TG 301B with the Substance;

You have also adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. and you have provided:

(ii) a supporting study by [redacted] (2007) corresponding to a ready biodegradability test performed according to OECD TG 301B with the source substance SCMI (CAS no. 869861-16-5).

We have assessed this information and identified the following issues:

A. Tests on substances must be conducted in accordance with the applicable OECD test guidelines or other internationally recognised test methods (Article 13(3) of REACH). For ready biodegradability testing OECD test guideline 301 and 310 are appropriate. For OECD 301B, the key parameters include:
   - an adequate description of the test material including purity, the presence (or not) of any co-formulant, the relative abundance of unreacted material(s),
   - information on the initial concentration of the test material in the test solution,
   - the description of the $ThCO_2$ calculation,
   - data on inorganic carbon (IC) content of the test substance suspension in the mineral medium is provided,
   - data on the inoculum concentration used to conduct the test is provided (mg/L SS and aprrox. cells/L),
   - CO_2 production data in tabular form.

   For study (i) above, you have not provided any of the information listed above and required by the OECD TG 301B.

   For study (ii) above, you have not provided information on purity and C-chain length distribution of the test material. You have not provided data on inorganic carbon (IC) content of the test substance suspension in the mineral medium, data on the inoculum concentration used to conduct the test and CO_2 production data in tabular form.

   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 301B study.

   In your comments on the draft decision you indicate your intention to update the robust study summaries for these studies.

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

Therefore the information requirement is not fulfiled.

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. **In vitro cytogenicity study in mammalian cells or in vitro micronucleus study (Annex VIII, Section 8.4.2.)**

An *in vitro* cytogenicity study in mammalian cells or an *in vitro* micronucleus study is a standard information requirement in Annex VIII to REACH.

You have adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. You have provided in your dossier:

(i) a key study by [redacted] (1991) corresponding to an *in vitro* chromosomal aberration assay performed according to OECD TG 476 with the analogue substance SCI (EC no. 263-052-5);
(ii) a key study by [redacted] (2008) corresponding to an *in vitro* mammalian cell micronucleus test (MNvit) performed according to OECD TG 487 with the analogue substance SCI (EC no. 263-052-5).

However, for the reasons detailed in the General considerations section the read-across approach to SCI is rejected.

Therefore, the information requirement is not fulfilled.

In your comments on the draft decision you indicate your intention to update the dossier with additional *in vitro* and *in vivo* data from "a structurally similar fatty acid isethionate salt and in silico QSAR data".

2. **Only if a negative result in Annex VII, Section 8.4.1. and Annex VIII, Section 8.4.2. is obtained, *in vitro* gene mutation study in mammalian cells (Annex VIII, Section 8.4.3.)**

An *in vitro* gene mutation study in mammalian cells is a standard information requirement in Annex VIII to REACH in case of a negative result in the *in vitro* gene mutation test in bacteria and the *in vitro* cytogenicity test.

In your dossier you provided a negative Ames test with the Substance and two negative cytogenicity studies with the source substance SCI. However, for the reasons detailed in the General considerations section the read-across approach to SCI is rejected. Therefore, for the *in vitro* cytogenicity study in mammalian cells or an *in vitro* micronucleus study there is a data gap for which information is requested in Appendix B1 of this decision. If the result of the requestd study is negative, an *in vitro* gene mutation study in mammalian cells must be requested.

You have adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. You have provided in your dossier:

(i) a key study by [redacted] (2007) corresponding to an *in vitro* gene mutation study in mammalian cells performed according to OECD TG 476 with the analogue substance

SCI (EC no. 263-052-5).

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

Therefore, the information requirement is not fulfilled.

In your comments on the draft decision you indicate your intention to update the dossier with additional *in vitro* and *in vivo* data from "a structurally similar fatty acid isethionate salt and in silico QSAR data".

Study design

To fulfil the information requirement for the Substance, both the *in vitro* mammalian cell gene mutation tests using the hprt and xprt genes (OECD TG 476) and the thymidine kinase gene (OECD TG 490) are considered suitable.

3. 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 adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. and you have provided in your dossier:

(i) a key study by [redacted] (2005) corresponding to a short-term toxicity study to fish performed according to EPA OPP 72-1 with the source substance SCMI (CAS no. 869861-16-5);
(ii) a supporting study by [redacted] (1984) corresponding to a short-term toxicity to fish performed similar to OECD TG 203 with the source substance SCI (EC no. 263-052-5).

We have assessed this information and identified the following issues:

A. Tests on substances must be conducted in accordance with the applicable OECD test guidelines or other internationally recognised test methods (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,
   - analytical monitoring of exposure concentrations is provided (including method description and results). Performance parameters should be reported (e.g. accuracy, precision, Limit of Detection, Limit of Quantification, specificity, working range).
   - the composition of the test medium and the preparation of test solutions is reported (including information on particulate matter, TOC, COD),
   - the spacing factor between test concentrations should not exceed 2.2,

   For study (i) above, you have not reported information on the purity of the test material or the presence of co-solvent (if any) and on the distribution of the C-chain length. You have not reported any information on the analytical monitoring of exposure concentrations. You define the test medium as "*reconstituted water with total hardness*

between 40 and 180 mg $CaCO_3$" but you have not provided information on the content in particulate matter, TOC and COD. You report that the spacing factor between exposure concentrations was 10.
For study (ii) above, you have you have not reported information on the C-chain length distribution of the test material. You report that an analytical monitoring of exposure was conducted using the "manual determination of anionic surface active materials (MBAS) by methylene blue spectrophotometric methods". 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 "*Unilever carbon filtered tap water*" but you have not provided information on the content in particulate matter, TOC and COD.

In your comments on the draft decision you indicate your intention to update the robust study summaries for these studies.

B. For the reasons detailed in the General considerations section the read-across approach to SCMI and SCI is rejected.

Therefore the information requirement is not fulfiled.

4. 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, or if the substance is highly insoluble in water.

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.3 above. Therefore, it cannot be used to waive the endpoint Hydrolysis as a function of pH.

Therefore, your adaptation is rejected and the information requirement is not fulfilled.

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

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

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

You have provided in your dossier a key study by Sydney (2009) corresponding to adsorption / desorption screening study according to EU method C.19 / OECD TG 121 with the Substance.

We have assessed this information and identified the following issue:

ECHA Guidance R.7a, Section R.7.1.15.3 specifies that the OECD TG 121/EU C.19 method is not suitable for some classes of chemical, for instance surface active substances.

The study you have provided to cover this information requirement was conducted according to OECD TG 121/EU C.19. Based on a study conducted according to OECD TG 115, you report that the surface tension of the Substance is 38.64 mN/m at 1.66 g/L and 20°C. Under section 3 of your technical dossier you report that the Substance is used in various consumer products with a technical function as surface active agent.

The information included in your dossier indicates that the substance has surface active properties. Therefore the results of the study conducted according to OECD TG 121/EU C.19 are not considered reliable.

In your comments on the draft decision you acknowledge that the existing OECD 121 (HPLC) data is not suitable given the ionic nature and surface-active properties of the Substance. You indicate your intention to provide new information for this information requirement.

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 by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. and you have provided in your dossier:

(i) a key study by [redacted] (2009) corresponding to a sub-chronic toxicity study performed according to OECD TG 408 with the analogue substance SI (EC no. 216-343-6).

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

You predict the properties of the Substance from the structurally similar substances listed in the Appendix on general considerations. However, the source substance SI used for this endpoint is not among the source substances listed in your justification.

In the read-across justification SI is mentioned in the following context: "*Metabolism would be expected to result in straight chain fatty acids (C8 to C18, innocuous components of the mammalian diet) and either sodium isethionate (SCI/SLI) or sodium methylisethionate (SLMI/SCMI/SDMI)*" and "*Sodium isethionate – likely to be the primary metabolite of SCI and SLI, and structurally very similar to sodium methylisethionate, the expected metabolite of SLMI, SCMI and SDMI – was reported to have a NOAEL of 200 mg/kg bw/day in a 90-day oral (gavage) study. There were no deaths or clinical signs in any rats administered 50, 200 or 1000 mg/kg bw/day for 91/92 days. High-dose animals were reported to have decreased body weights, a variety of altered haematological parameters (including increased total bilirubin), and histopathological changes to the liver and spleen. Spleen weights were also increased at the top dose.*"

ECHA understands that you predict the properties of the Substance using a read-across hypothesis which is based 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.

We have assessed this information and identified the following issue:

A. As indicated above, your read-across hypothesis is based on the (bio)transformation of the Substance into an analogue of the presumed sole metabolite of the Substance. This analogue metabolite is the proposed source substance. In this context, information characterising the rate and extent of the hydrolysis of the Substance is necessary to confirm the rapid formation of the sole proposed hydrolysis product (i.e. SI analogue) and to demonstrate that the exposure to the parent compound is negligible.

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

The available data indicates a deviation from your claimed similar rapid hydrolysis of the ester bond *in vivo*. The data show that there is significant exposure to the parent substance. Furthermore, the provided data are not for the target but for yet other analogue and the relevance of the data produced with these substances for the Substance was not discussed. Therefore, you have not demonstrated and justified that the Substance rapidly form one common (bio)transformation product and that no significant exposure to the parent compound is expected.

B. Annex XI, Section 1.5 of the REACH Regulation states that "physicochemical properties, human health effects and environmental effects or environmental fate may be predicted from data for reference substance(s)". For this purpose "it is important to provide supporting information to strengthen the rationale for the read-across" (Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of Chemicals, Section R.6.2.2.1.f). The set of supporting information should allow to verify the crucial aspects of the read-across hypothesis and establish that the properties of the Substance can be predicted from the data on the source substance(s).

When a read-across hypothesis is based on the assumption that the Substance rapidly form (bio)transformation products similar to the source substance and cause the same type of effect(s). , relevant, reliable and adequate information allowing to compare the properties of the Substance is necessary to confirm that both substances cause the same type of effects. Such information can be obtained, for example, from bridging studies of comparable design and duration for the target and source substances.

Similar toxicity is claimed between the target and the source substances. However, no toxicology data are available for the target for any endpoint except an inconclusive eye irritation study and an Ames study. Therefore, a direct comparison of the toxicological potency between the target and the source is not possible. Furthermore, with the exception of a NOEL from a 90d-study and two genetoxicity study results, the toxicology data for the source SCMI, which has a methyl group similar to the target substance, are not provided in order to allow to understand the contributin of the methyl group to toxicity. In the read-across justification, for the toxicological properties you have provided information only on esters of medium-long chain fatty acids isethionate. You have not provided information on esters of medium-long chain fatty acids methyl isethionate.

Therefore, the data set reported in the technical dossier does not include relevant, reliable and adequate information to support your read-across hypothesis. In the absence of such information, you have not established that the Substance and the proposed source are likely to have similar properties. Therefore you have not provided sufficient supporting information to strengthen the rationale for the read-across.

As explained above, you have not 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.

Therefore, the information requirement is not fulfilled.

In your comments on the draft decision you indicate your intention to update the dossier to include repeat dose toxicity data for a structurally similar fatty acid isethionate salt and to improve the scientific rationale for the read-across.

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 granular solid not expected to lead to inhalation hazard.

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

Pre-natal developmental toxicity study is a standard information requirement in Annex IX to REACH.

You have adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. and you have provided in your dossier:

(i) a key study by [redacted] (2008) corresponding to a pre-natal developmental toxicity study in a first species (rat) performed according to OECD TG 414 with the analogue substance Fatty acids, c12-18 and c18-unsatd., 2-sulfoethyl esters (EC no. 287-024-7)

We have assessed this information and identified the following issue:

Annex XI, Section 1.5 requires that whenever read-across is used adequate and reliable documentation of the applied method must be provided. Such documentation must provide a justification for the read-across including a hypothesis, explanation of the rationale for the prediction of properties and robust study summary(ies) of the source study(ies).[3]

You have provided a study conducted with other substances than your Substance in order to comply with the REACH information requirements. You have not provided documentation as to why this information is relevant for your Substance.

In the absence of such documentation, ECHA cannot verify that the properties of your Substance can be predicted from the data on the source substance.

Therefore, the information requirement is not fulfilled.

[3] Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of Chemicals, Section R.6.2.6.1

In your comments on the draft decision you indicate your intention to update the dossier to improve the scientific rationale for the read-across and to include additional supporting data for a weight of evidence approach.

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: "*In accordance with column 2 of REACH annex X, long term toxicity to fish testing does not need to be conducted as the chemical safety assessment does not indicate a need for further investigation*".

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 to 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.1, A.2 and B.3, 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 (38.64 mN/m at 1.66 g/L and 20°C), is used in various consumer products with a technical function as surface active agent and is ionisable, indicating high adsorptive properties.

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 Gore (2010) corresponding to simulation test – Activated sludge unit according to OECD TG 303A with the source substance SCI (EC no. 263-052-5).

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 SCI 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 you have provided is based on OECD TG 303A which is a test to simulate degradation in an aerobic sewage treatment plant and is not 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.

Therefore these 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 direct and indirect exposure of the aquatic compartment is unlikely*".

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 direct and indirect exposure of the aquatic compartment is unlikely. As specified in ECHA Guidance R.7c, Section R.7.10.4.5, bioaccumulation is a fundamental part of the assessment of the hazard and fate of a substance and therefore testing may only be omitted on exposure grounds under exceptional circumstances. Such circumstances include cases where it can be reliably demonstrated (by measurement or other evidence) that there is no release to the environment at any stage in the life cycle.

You have not provided any justification as to why exposure of the aquatic compartment is unlikely.

In your CSR you report wide dispersive uses including consumer uses (e.g. various detergent application, cosmetics and biocidal products). Therefore exposure of the aquatic compartment cannot be ruled out and your adaptation is rejected.

Therefore, your adaptation does not fulfil the information requirement.

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: Reasons for the requests to comply with Annex X of REACH

Under Articles 10(a) and 12(1) of REACH, a technical dossier at a tonnage abve 1000 tonnes per year must contain, as a minimum, the information specified in Annexes VII to X to REACH.

1. Pre-natal developmental toxicity study (Annex X, Section 8.7.2.) in a second species

Pre-natal developmental toxicity (PNDT) studies (OECD TG 414) in two species is a standard information requirement under Annex X to REACH.

You have adapted the standard information requirement according to Annex XI, Section 1.2. Weight of evidence of REACH.

In support your adatation, you have provided the following sources of information:

(i) OECD 421 reproductive screening study on the read across substance Fatty acids, C12-18 and C18-unstaurated, 2-sulfoethyl esters, sodium salt
(ii) OECD 408 (90 day study) on the metabolite sodium 2-hydroxyethanesulfonate CAS No 1562-00-1 (sodium isethionate)
(iii) OECD 414 pre-natal developmental study in rats on the read across substance Sodium lauryl isethionate (Fatty acids, C12-18 and C18-unsaturated, 2-sulfoethyl esters, sodium salt CAS No 85408-62-4)
(iv) Toxicokinetic information on an analogue substance indicating low adsorption followed by rapid metabolism

Based on the presented sources of information, you argue that the available data gives sufficient information to conclude on the 2nd species developmental toxicity because "*Multiple reprotox studies indicate no adverse effect so waived on animal welfare grounds*" (a).
Annex XI, Section 1.2 states that there may be sufficient weight of evidence from several independent sources of information leading to assumption/conclusion that a substance has or has not a particular dangerous (hazardous) property, while information from a single source alone is insufficient to support this notion.

According to ECHA Guidance R.4.4, a weight of evidence adaptation involves an assessment of the relative values/weights of different sources of information submitted. The weight given is based on the reliability of the data, consistency of results/data, nature and severity of effects, and relevance of the information for the given regulatory information requirement. Subsequently, relevance, reliability, consistency and results of these sources of information must be balanced in order to decide whether they together provide sufficient weight to conclude that the Substance has or has not the (dangerous/hazardous) property investigated by the required study.

Annex XI, section 1.2 requires that adequate and reliable documentation is provided to describe your weight of evidence approach.

However, you have not submitted any explanation why the sources of information provide sufficient weight of evidence leading to the conclusion/assumption that the Substance has or has not a particular dangerous property.

In spite of this critical deficiency, ECHA has nevertheless assessed the validity of your adaptation.

In order to allow concluding on no prenatal developmental toxicity in two species for the Substance in a weight of evidence adaptation, the information justification must cover the key parameters foreseen to be investigated in an OECD TG 414 study in two species. The key parameters of this test guideline include external, skeletal and soft tissue alterations (variations and malformations) in developing animals.

ECHA has assessed to what extent the information submitted enables a conclusion of hazardous properties for reproduction and identified the following deficiencies:

The OECD 408 study and the toxicokinetic information do not provide information in developing animals and these studies are therefore not relevant for the weight of evidence on pre-natal developmental toxicity.

Although the study OECD TG 421 involves developing animals it does not investigate structural malformations and variations as required in a pre-natal developmental toxicity study (OECD TG 414).

From sources of information, the OECD TG 414 study provide information on developmental toxicity on one species only (rat). While this study is relevant for the information requirement for a developmental toxicity study on a first species, it is not relevant for the information requirement for a developmental toxicity study on a second species.

Furthermore, you provided the information from OECD TG 414 with a read-across source substance and this approach is not reliable has already explained under Appendix C.2. Even is it would be considered reliable enough, a weight of evidence adaptation cannot be based on only one soruce of information according to Annex XI, Section 1.2.

Your weight of evidence adaptation does not include relevant or reliable sources of information to conclude on the property of prenatal developmental toxicity on a second species. Therefore your adaptation is rejected and the information requirement is not fulfilled.

In your comments on the draft decision you indicate your intention to waive this information requirement with an updated adaptation in accordance with REACH Annex X, Section 8.7, Column 2.

Study design

A PNDT study according to the OECD TG 414 study should be performed in rabbit or rat as the preferred second species, depending on the species tested in the first PNDT study (request C.2. in this decision).

The study shall be performed with oral (ECHA Guidance R.7a, Section R.7.6.2.3.2.) administration of the Substance.

2. Long-term toxicity to sediment organisms (Annex X, Section 9.5.1.)

Long-term toxicity to sediment organisms is a standard information requirement in Annex X to REACH.

You have adapted this information requirement Annex IX, Section 9.1., Column 2 with the following justification: "*In accordance with column 2 of REACH Annex X, sediment toxicity*

testing does not need to be conducted as the chemical safety assessment does not indicate a need for further investigation".

You relied on the results of short-term aquatic toxicity data included in your dossier to extrapolate the PNECs sediment using the equilibrium partitioning method.

We have assessed this information and identified the following issues:

A. ECHA Guidance R.10, Section R.10.5.2.1. specifies that for compounds with a log Kow greater than 5 or with a corresponding adsorption or binding behaviour not triggered by the lipophilicity (e.g. log Kow) of the substance but by other mechanisms (e.g. ionisable substances, surface active substances, substances forming covalent bound to sediment, components like e.g. aromatic amines) the equilibrium method is used in a modified way. In such cases, the PECsed/PNECsed ratio is increased by a factor of 10.

   Based on a study conducted according to OECD TG 115, you report that the surface tension of the Substance is 38.64 mN/m at 1.66 g/L and 20°C. Under section 3 of your technical dossier your report that the Substance is used in various consumer products with a technical function as surface active agent.

   The information in your dossier indicates that the Substance is ionisable and surface active. You have not applied the extra assessment factor of 10 in the calculation of the PECsed/PNECsed ratios. Therefore your CSR currently underestimates the risks to the sediment compartment by a factor of 10.

B. As specified in Annex X, Section 9.5.1., Column 2, a long-term toxicity to study on sediment organisms 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 to extrapolate the PNECs sediment using the equilibrium partitioning method and the outcome of the exposure assessment showing risk characterisation ratios (RCRs) below 1 for the freshwater and marine sediment compartments. The highest RCR reported for freshwater sediment in your CSR is [redacted].

   As specified in request A.2, A.3 and B.3, 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.

Furthermore as explained under issue A above, You have not applied the extra assessment factor of 10 in the calculation of the PECsed/PNECsed ratios and hence your CSR currently underestimates the risks to the sediment compartment by a factor of 10.

Therefore your Chemical Safety Assessment does not demonstrate that the risks of the Substance are adequately controlled.

Therefore , your adaptation is according to Annex X, Section 9.5.1., Column 2 is rejected and the information requirement is not fulfilled.

In your comments on the draft decision you indicate your intention to revise the chemical safety assessment (CSA) and derive a new PNECsed (EPM). You also state your intention to apply an additional assessment factor of 10 to this value as advocated by the ECHA guidance for ionisable/surface active substances. If, based on the updated CSA the risk characterisation ratio (RCR) for the sediment compartment is < 1 then you intend to waive experimental testing for long-term toxicity in sediment organisms in accordance with REACH Annex X, Section 9.5.1, Column 2.

Study design

The Sediment-water Chironomid toxicity using spiked sediment (OECD TG 218), Sediment-water Lumbriculus toxicity test using spiked sediment (OECD TG 225) and Sediment-Water Chironomid Life-Cycle Toxicity Test Using Spiked Sediment (OECD TG 233) are in principle each considered capable of generating information appropriate for the fulfilment of the information requirements for sediment long-term toxicity testing. ECHA is not in a position to determine the most appropriate test protocol, since this decision is dependent upon species sensitivity, substance properties and uses. ECHA considers that it is your responsibility to choose the most appropriate test protocol and to give a justification for the choice. You may carry out more than one of the sediment tests listed above if you consider that further testing is required.

Appendix E: 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.

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 and 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 F: Observations and technical guidance

1. The information requirement under Section 8.7.1. and 8.7.3. of Annex X to REACH (Extended one-generation reproductive toxicity study, EOGRTS) is not addressed in this decision, because the information from the Sub-chronic toxicity study (90-day), requested in the present this decision, is relevant for the design of the EOGRTS.

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

3. 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.

4. 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'[4].

5. Test material

   Selection of the test material(s)

   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"[5].

[4] https://echa.europa.eu/practical-guides
[5] https://echa.europa.eu/manuals

6. 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.

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

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)[7]

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.

[6] https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment
[7] 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.10 (version 1.0, May 2008), referred to as ECHA Guidance R.10 in this decision.

PBT assessment
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[8]
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.

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

Appendix G: 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.