EUROPEAN CHEMICALS AGENCY

Helsinki, 27 October 2016

Addressee: [redacted]

Decision number: CCH-D-2114347491-50-01/F
Substance name: [3R-(3α,3aβ,7β,8aα)]-1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)ethan-1-one
EC number: 251-020-3
CAS number: 32388-55-9
Registration number: [redacted]
Submission number: [redacted]
Submission date: 10.04.2013
Registered tonnage band: 100-1000 tonnes per year

DECISION ON A COMPLIANCE CHECK

Based on Article 41 of Regulation (EC) No 1907/2006 (the 'REACH Regulation'), ECHA requests you to submit information on

1. **Name(s) in the IUPAC nomenclature or other international chemical name(s) (Annex VI, Section 2.1.1.) of the registered substance;**
   - **Chemical name and EC and CAS entry which are consistent with each other and consistent with the composition reported in section 1.2 of the dossier**
2. **Composition of each substance (Annex VI, Section 2.3.)**

You are required to submit the requested information in an updated registration dossier by **3 February 2017**. You shall also update the chemical safety report, where relevant.

The reasons of this decision are set out in Appendix 1. The procedural history is described in Appendix 2. Advice and further observations are provided in Appendix 3.

The scope of this compliance check decision is limited to the standard information requirement(s) of Annex VI, Section 2 of the REACH Regulation.

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, shall 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.

Authorised[1] by Ofelia Bercaru, Head of Unit, Evaluation E3

[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 1: Reasons

1. Name(s) in the IUPAC nomenclature or other international chemical name(s) (Annex VI, Section 2.1.1.);

Pursuant to Article 10(a)(ii) of the REACH Regulation, the technical dossier shall contain information on the identity of the substance as specified in Annex VI, Section 2 of the REACH Regulation. In accordance with Annex VI, Section 2 the information provided shall be sufficient to enable the identification of the registered substance.

In line with the 'Guidance for identification and naming of substances under REACH and CLP' (Version: 1.4, June 2016), referred to as "the Guidance" hereinafter, mono-constituent substances are well defined substances in which one constituent is present at a concentration ≥80% (w/w).

According to paragraph 4.2 of the Guidance, well defined mono-constituent substances are defined by their qualitative and quantitative composition and for this type of substances the following applies:

- All the impurities present at ≥ 1 % shall be identified and reported individually;

and

- All the impurities relevant for the classification and/or PBT assessment shall be identified and reported individually.

For each constituent, including the main constituent and any impurity, the typical, minimum and maximum concentration level shall be specified.

According to the Guidance, substances that cannot be sufficiently identified by their chemical composition, because:

- The number of constituents is relatively large and/or

- The composition is, to a significant part, unknown and/or

- The variability of composition is relatively large or poorly predictable

are normally regarded as substances of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB).

The information provided on the name and identifiers of any well defined or UVCB substance needs to be consistent with the composition and the supporting analytical data included in the registration dossier.

You identified the registered substance as a mono-constituent substance and assigned EC and CAS entries and chemical name corresponding to [redacted]" to the registered substance.

The composition information you reported in the IUCLID dossier includes:

- one clearly identified predominant constituent, the concentration levels of which vary from [redacted]% (w/w) to [redacted]% (w/w).
- 7 "impurities", the individual upper concentration levels of which exceed [redacted]% (w/w). These constituents have been generically reported as: Isomer "X" of acetyl cedrene. For two of these impurities the individual upper concentration level amounts to [redacted]% (w/w) and [redacted]% (w/w) respectively.
- 19 unknown "impurities" with individual concentration values <[redacted]% and which cumulative upper concentration level corresponds to [redacted]% (w/w).

The registration dossier includes the following information on the manufacturing of the registered substance: You stated that the registered substance "[redacted] Details on other starting materials used and steps carried out for the synthesis and isolation of the substance have not been reported.

On the basis of the above information provided:

- The composition of the registered substance does not include any constituent at concentration levels ≥80% (w/w) therefore it does not fulfil the above-mentioned rule of thumb set for defining mono-constituent substances
- Part of the composition of the registered substance is unknown and has not been clearly identified as expected for well defined substances
- The variability of the concentration range values reported for the predominant constituent corresponds to around [redacted]%
- In situations where the predominant constituent would be present in the substance at the lower concentration level, namely at [redacted]% (w/w)
    - The composition of the registered substance would remain mostly unknown or generically described.
    - Up to two thirds of the composition would not be represented by the name currently specified for identifying the registered substance

You provided a justification for registering the substance as a mono-constituent substance and deviating from the 80% rule explained in the Guidance.

ECHA notes the following in relation to the justification provided:

a. Your justification explains that the registered substance cannot be regarded as a well defined multi-constituent substance because only one constituent is present in the substance at concentration values >[redacted]%

   ECHA agrees with you that defining the registered substance as a multi-constituent substance would not be considered appropriate.

b. You point out that, according to the Guidance, deviation from the 80% rule is acceptable when appropriately justified.

You also provide a justification for deviating from the 80% rule stating "....only the MCK with [redacted]% content is marketable and meet the consumer requirement, no product with over 80% purity is distributed in the real supply chain and can be regarded as the "mono-constituent substance" reference for comparison, in terms of physicochemical and hazard profile properties, according to the statement set out with the Guidance."

Indeed, according to paragraph 4.2.1.2 of the Guidance, if the main constituent of a substance is <80%, deviation from the 80% rule can be justified. Justifying is possible if the substance can be shown to have similar physico-chemical properties and the same hazard profile as the other mono-constituent substance with the same identity that fulfil the 80% rule.

In order to justify a deviation from the 80% rule, registrants need to define first the pre-conditions for applying such a deviation. In the justification you provided, however, the mono-constituent substance you wish to refer to is actually not available and as a consequence no physical-chemical property and hazard profile can be compared.

Therefore for this substance the pre-conditions for deviating from the 80% rule explained above are not fulfilled. As a consequence such a deviation cannot be applied.

c. You explained that the approach followed for identifying the registered substance is based on the historical use of the CAS identifier. The CAS entry (32388-55-9) used, which describes specifically the predominant constituent and would be appropriate for identifying a mono-constituent substance, has been used in the past for identifying the registered substance.

ECHA understands that maintaining the CAS identifier formerly used to identify the substance is of practical convenience to you. However ECHA underlines that accurate identification of substances is a pre-requisite to REACH processes. Therefore, considering that the CAS identifier is an essential element of substance identification, ensuring its appropriateness is crucial. As explained above, the information given on the composition section of the IUCLID dossier rather refers to a UVCB substance. The CAS entry currently reported is not appropriate for identifying a UVCB substance.

d. You stated that the concentration levels reported for the predominant constituent depend on the variability of the composition of the starting material used for its production and therefore are inherent to the manufacturing process.

Such information indicates that the variability of the composition of the substance is poorly predictable and therefore it supports the above reasoning in relation to the identification of the registered substance as of UVCB.

On the basis of the above reasoning ECHA concludes that the composition as currently reported is not consistent with the provided EC/CAS entries and chemical name.

Therefore you are requested to clarify this inconsistency by selecting the correct substance type and the corresponding chemical identifiers for the registered substance. ECHA foresees two possibilities:

(i). If the substance subject to this registration is a UVCB substance, you shall note that information required to be provided on the naming of UVCB substances such as the registered substance shall consist of two parts: (1) the chemical name and (2) a more detailed description of the manufacturing process, as indicated in chapter 4.3 of the Guidance.

(1) Chemical name:

The chemical name shall be representative of the source and process used for the manufacturing of the registered substance and should follow the generic format "Reaction products of [name of the starting materials]". You are accordingly requested to provide a chemical name corresponding to the specific substance covered in this registration.

(2) Description of the manufacturing process:

A detailed description of the manufacturing process shall be included in the registration dossier. For each step, the relevant process parameters (such as identity and ratio of reactants, operating parameters (temperature and pressure), etc.) shall be specified. Information on processing steps applied to isolate the manufactured substance and any purification/fractionation steps used shall be provided as well.

Furthermore you shall replace the CAS entry (CAS n. 32388-55-9) currently assigned to the registered substance by an appropriate CAS name and CAS number, if available. In order to maintain a link to CAS number 32388-55-9 you may however report the current CAS entry as "Related CAS information" in the dossier. You are also requested to revise the molecular and structural identifiers reported in IUCLID section 1.1 as these are not representative of the registered substance.

(ii). If the substance subject to this registration has a different composition than the composition currently reported in the IUCLID dossier and is a well-defined substance, you shall

- Ensure that the chemical name provided for the registered substance is in accordance with the naming conventions specified in chapter 4.2 of the Guidance and is appropriately representing of the composition of the registered substance.
- Revise the compositional information such that
  - All the impurities present at ≥ 1 % are identified and reported individually; And
  - All the impurities relevant for the classification and/or PBT assessment are identified and reported individually.
- Ensure that the analytical data support the identity and compositional information of the registered well-defined substance.

As for the reporting of the information in IUCLID,

- the chemical name shall be indicated in the "IUPAC name" field in IUCLID section 1.1.
- the manufacturing process description shall be specified in the Description filed of the reference substance assigned in IUCLID section 1.1.
- The CAS number and CAS name shall be reported under the "CAS information" header in IUCLID section 1.1.

Further technical details on how to report the identifiers of UVCB substances in IUCLID are available in paragraphs 2.1 of the Data Submission Manual 18 on the ECHA website.

You shall ensure that the molecular and structural information specified in IUCLID section 1.1 and the composition indicated in IUCLID section 1.2 are consistent with the chemical name and CAS number and CAS name assigned to the registered substance.

You shall note that the registration is currently linked to the EC number referring to 251-020-3. In case the current identifiers are not appropriate to describe the registered substance, you should not remove or modify at this stage the EC number for technical reasons, the registration being linked to that number in REACH-IT. To ensure unambiguous identification of the registered substance, you shall however indicate, in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The EC number 251-020-3 currently assigned does not specifically correspond to the registered substance. This identifier cannot be modified or deleted at this stage in the present registration update for technical reasons". You shall also specify, in the same "Remarks" field, any available and appropriate EC number for the substance.

You should note that ECHA has established a process, subject to certain conditions, enabling registrants to adapt the identifier of an existing registration, while maintaining the regulatory rights already conferred to the substance concerned.
However, pending the resolution of all the incompliances highlighted in the present decision, the adaptation of the identifier can only be effective once ECHA is at least in a position to establish unambiguously the identity of the substance intended to be covered by you with this registration. Should the information submitted by you as a result of the present decision enable ECHA to identify the substance unambiguously, the process of adapting the identifier will be considered relevant. In that case, ECHA will inform you in due time as to when the identifier adaptation process shall be initiated.

In any case, you should note that the application of the process of adapting the identifier does not affect his obligation to fulfil the requirements specified in this decision.

2. Composition of the substance (Annex VI, Section 2.3.);

Pursuant to Article 10(a)(ii) of the REACH Regulation, the technical dossier shall contain information on the identity of the substance as specified in Annex VI, Section 2 of the REACH Regulation. In accordance with Annex VI, Section 2 the information provided shall be sufficient to enable the identification of the registered substance.

The substance composition corresponds to the chemical representation of what the substance consists of and is therefore an essential part of substance identification and the cornerstone of all the REACH obligations.

Annex VI, section 2.3. of the REACH Regulation requires that each registration dossier contains sufficient information for establishing the composition of the registered substance and therefore its identity.

As explained under section (a) Name or other identifier of the substance the information given in the composition section of the IUCLID dossier indicates that the registered substance should be regarded as a UVCB substance.

According to ECHA Guidance chapter 4.3, you should note that, for UVCB substances, the chemical composition and identity of the constituents should be given as far as known and the following applies:

- All constituents present in the substance with a concentration of ≥ 10 % shall be identified and reported individually;

- All known constituents, including isomers, and constituents relevant for the classification and/or PBT assessment of the registered substance shall be identified and reported individually; and

- Unknown constituents shall be identified as far as possible by a generic description of their chemical nature.

For each constituent or group of constituents, the typical, minimum and maximum concentration levels shall be specified. Whilst for UVCB substances you are not required to identify each single constituent present in the composition of the registered substance, having as precise information as possible on the composition of a registered substance is an essential element of substance identification.

For a well-defined substance, the follwing information is required:

- All the impurities present at ≥ 1 % must be identified and reported individually; and

- All the impurities relevant for the classification and/or PBT assessment must be identified and reported individually.

ECHA notes that the composition reported in the IUCLID dossier includes clear information on the identity of one constituent present in the substance at concentration levels varying form [redacted]% (w/w) to [redacted]% (w/w). Other constituents are reported as unknown or have been generically identified as Isomer "X" of acetyl cedrene. No further information is given on the identity of these constituents.

As no information was provided on the identity of these isomers, the composition is not explained with respect to the constituents present in the registered substance.

Based on the fact that you manufacture the substance, choose the starting materials, and control the process parameters, you can provide more information on these constituents

In line with the above, you shall report the missing compositional information of the registered substance.

More specifically, in the compositional information of the IUCLID dossier you shall ensure the following:

- All constituents present in the substance with a concentration of ≥ 10 % are identified and reported individually;

- All known constituents, including isomers, and constituents relevant for the classification and/or PBT assessment of the registered substance are identified and reported individually; and

- Unknown constituents are identified as far as possible by a generic description of their chemical nature. As explained above you shall provide a more precise description of the isomers present in the composition of the registered substance. Whilst it is your responsibility to determine the appropriate methods for the identification of the registered substance, ECHA would like to draw the attention on the following:
  Considering the complexity of the composition of the registered substance, you may, if appropriate, rely on bibliographical reference regarding the composition in terms of the isomeric constituents present in the substance (e.g. peer reviewed data from the literature) and knowledge on the composition of the starting material and the reactions taking place during manufacturing, to fill the current data gap on the composition. Such approach to derive the composition should be described in the dossier so that it can be reproduced.

As explained under point 1 of the present decision, should the registered substance be identified as a well-defined substance you shall revise the compositional information such that

- All the impurities present at ≥ 1 % are identified and reported individually; And

- All the impurities relevant for the classification and/or PBT assessment are identified and reported individually.

In addition you shall ensure that the analytical data support the identity and compositional information of the registered well-defined substance.

Regarding how to report the composition of the registered substance in IUCLID, the following applies: you shall indicate the composition of the registered substance in IUCLID Section 1.2. For each constituent required to be reported individually, the IUPAC name, CAS name and CAS number (if available), molecular and structural formula, as well as the minimum, maximum and typical concentration, shall be reported in the appropriate fields in IUCLID. For the other constituents to be reported under a generic description, a generic chemical name describing the group of constituents, generic molecular and structural information (if applicable), as well as the minimum, maximum and typical concentration, shall be reported in the appropriate fields in IUCLID.

Further technical details on how to report the composition of UVCB and well defined substances in IUCLID are available in paragraphs 2.1 and 2.2 of the Data Submission Manual 18 on the ECHA website.

Appendix 2: Procedural history

For the purpose of the decision-making, this decision does not take into account any updates of your registration after the date when the draft decision was notified to you under Article 50(1) of the REACH Regulation.

The compliance check was initiated on 25 September 2015.

The decision making followed the procedure of Articles 50 and 51 of the REACH Regulation:

ECHA notified you of the draft decision and invited you to provide comments.

ECHA did not receive any comments by the end of the commenting period.

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

As no amendments were proposed, ECHA took the decision according to Article 51(3) of the REACH Regulation.

Appendix 3: Further information, observations and technical guidance

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

2. Failure to comply with the request(s) in this decision, or to fulfil otherwise the information requirement(s) with a valid and documented adaptation, will result in a notification to the enforcement authorities of your Member State.