Lauric acid

(CAS-no. 143-07-7)

Doc III-A

Applicant:
Dr. R. Pfleger Chemische Fabrik GmbH

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Section A1 Applicant

Annex Point IIA.1

1.1 Applicant

Name: Dr. R. Pfleger Chemische Fabrik GmbH
Address: D-96045 Bamberg
Telephone: 0951/6043-0
Fax number: 0951/6043-29
E-mail address: info@dr-pfleger.de

1.2 Manufacturer of Active Substance (if different)

Name: Acidchem International SDN.BHD
Address: P.O. Box 237, 12720 Butterworth, Penang, Malaysia
Contact over the supplier: [redacted]

Location of manufacturing plant:
Acidchem International SDN.BHD, 2411. Lrg. Perusahaan Satu, Prai Industrial Complex, 13600 Prai, Penang, Malaysia

1.3 Manufacturer of Product(s) (if different)

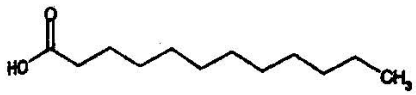
1) Product 1

Dr. R. Pfleger Chemische Fabrik GmbH
see above 1.1 Applicant

Section A2 Identity of Active Substance

Subsection
(Annex Point)

Official use only

2.1	**Common name (IIA2.1)**	Lauric acid (IUPAC), Laurostearic acid, Dodecoid acid
2.2	**Chemical name (IIA2.2)**	Dodecanoic acid
2.3	**Manufacturer´s development code number(s) (IIA2.3)**	Art. No. 6150
2.4	**CAS No and EC numbers (IIA2.4)**	
2.4.1	**CAS-No**	143-07-7
	Isomer 1	There is no isomerism of lauric acid kown.
2.4.2	**EC-No**	205-582-1
	Isomer 1	There is no isomerism of lauric acid kown.
2.4.3	**Other**	-
2.5	**Molecular and structural formula, molecular mass (IIA2.5)**	
2.5.1	**Molecular formula**	$C_{12}H_{24}O_2$
2.5.2	**Structural formula**	
2.5.3	**Molecular mass**	M_r 200.32
2.6	**Method of manufacture of the active substance (IIA2.1)**	Palm oil, palm kernel oil or RDB stearine are used as starting material. By hydrolysis of water fat splitting is conducted: the fat reacts with water to yield fatty acids and glycerine. The crude fatty acids are purified by fractional distillation. The destillation produces fatty acids of high quality. The results are fatty acids as e.g. lauric acid.
2.7	**Specification of the purity of the active substance, as appropriate (IIA2.7)**	g/kg [redacted] lauric acid; g/l [redacted] lauric acid; % w/w [redacted] lauric acid; % v/v -
	Content of lauric acid in different batches (determined by the applicant according to Doc. III-A, 4.1)	Batch 37077 [redacted]; 40561 [redacted]; 42731 [redacted]; 43080 [redacted]; 43256 [redacted]
	Average content of lauric acid	[redacted]

Section A2 Identity of Active Substance

2.8	**Identity of impurities and additives, as appropriate (IIA2.8)**	For identified impurities see separate standard format In addition: [redacted] [redacted]
2.8.1	**Isomeric composition**	There is no isomerism of lauric acid kown.
2.9	**The origin of the natural active substance or the precursor(s) of the active substance (IIA2.9)**	Natural origin of palm oil, palm kernel oil or RDB Stearine

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	*Give date of action*
Materials and methods	*State if the applicants version is acceptable or indicate relevant discrepancies referring to the (sub) heading numbers and to applicant's summary and conclusion.*
Conclusion	*Adopt applicant´s version or include revised version*
Reliability	*Based on the assessment of the method include appropriate reliability indicator*
Acceptability	acceptable / not acceptable *(give reasons if necessary, e.g. if a study is acceptable despite a poor reliability indicator). Discuss the relevance of deficiencies.*
Remarks	
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant´s summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Section A2.8 Identity of impurities and additives (active substance)

Annex Point IIA II2.8 Capric acid

Official use only

Subsection

2.8.1.1 Common name Capric acid

2.8.1.2 Function [redacted].

2.8.2 IUPAC name Decanoic acid

2.8.3 CAS-No 334-48-5

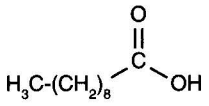
2.8.4 EC-No 206-376-4

2.8.5 Other

CIPAC Not listed by CIPAC.

2.8.6 Molecular formula $C_{10}H_{20}O_2$

2.8.7 Structural formula



2.8.8 Molecular mass 172.26

	g/kg	g/l	% w/w	% v/v
2.8.9 Concentration of the impurity or additive	[redacted]	[redacted]	[redacted]	-
Content of capric acid in different batches	[redacted]	[redacted]	[redacted]	Batch 37077
	[redacted]	[redacted]	[redacted]	40561
	[redacted]	[redacted]	[redacted]	42731
	[redacted]	[redacted]	[redacted]	43080
	[redacted]	[redacted]	[redacted]	43256
Average content of capric acid	[redacted]	[redacted]	[redacted]	

Section A2.8 Identity of impurities and additives (active substance)

Annex Point IIA2.8

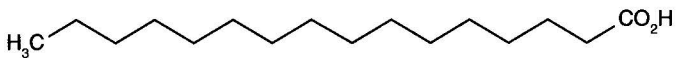
	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	*Give date of action*
Materials and methods	*State if the applicants version is acceptable or indicate relevant discrepancies referring to the (sub) heading numbers and to applicant's summary and conclusion.*
Conclusion	*Adopt applicant´s version or include revised version*
Reliability	*Based on the assessment of the method include appropriate reliability indicator*
Acceptability	acceptable / not acceptable *(give reasons if necessary, e.g. if a study is acceptable despite a poor reliability indicator). Discuss the relevance of deficiencies.*
Remarks	
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant´s summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Section A2.8 Identity of impurities and additives (active substance)

Annex Point IIA II2.8 n-Hexadecanoid acid

Official use only

Subsection

2.8.1.1	**Common name**	n-Hexadecanoic acid
2.8.1.2	Function	[redacted]
2.8.2	**IUPAC name**	Palmitic acid
2.8.3	**CAS-No**	57-10-3
2.8.4	**EC-No**	200-312-9
2.8.5	**Other**	
	CIPAC	Not listed by CIPAC.
2.8.6	**Molecular formula**	$C_{16}H_{32}O_2$
2.8.7	**Structural formula**	

2.8.8	**Molecular mass**	256.42			
2.8.9	**Concentration of the impurity or additive**	g/kg	g/l	% w/w	% v/v
		[redacted]	[redacted]	[redacted]	-
	Content of n-Hexadecanoic acid in different batches	[redacted]	[redacted]	[redacted]	Batch 37077 40561 42731 43080 43256
	Average content of Hexadecanoic acid	[redacted]	[redacted]	[redacted]	

Section A2.8 Identity of impurities and additives (active substance)

Annex Point IIA2.8

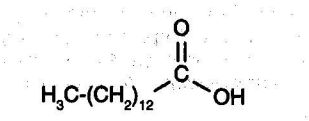
	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	*Give date of action*
Materials and methods	*State if the applicants version is acceptable or indicate relevant discrepancies referring to the (sub) heading numbers and to applicant's summary and conclusion.*
Conclusion	*Adopt applicant´s version or include revised version*
Reliability	*Based on the assessment of the method include appropriate reliability indicator*
Acceptability	acceptable / not acceptable *(give reasons if necessary, e.g. if a study is acceptable despite a poor reliability indicator). Discuss the relevance of deficiencies.*
Remarks	
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant´s summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Section A2.8 Identity of impurities and additives (active substance)

Annex Point IIA II2.8 Myristic acid

Official use only

Subsection

2.8.1.1	**Common name**	Myristic acid
2.8.1.2	Function	[redacted].
2.8.2	**IUPAC name**	Myristic acid
2.8.3	**CAS-No**	544-63-8
2.8.4	**EC-No**	208-875-2
2.8.5	**Other**	
	CIPAC	Not listed by CIPAC.
	Name	Tetradecanoic acid
2.8.6	**Molecular formula**	$C_{14}H_{28}O_2$
2.8.7	**Structural formula**	
2.8.8	**Molecular mass**	228.36

2.8.9 Concentration of the impurity or additive

	g/kg	g/l	% w/w	% v/v
	[redacted]	[redacted]	[redacted]	

Content of myristic acid in different batches

	g/kg	g/l	% w/w	% v/v
Batch 37077	[redacted]	[redacted]	[redacted]	
Batch 40561	[redacted]	[redacted]	[redacted]	
Batch 42731	[redacted]	[redacted]	[redacted]	
Batch 43080	[redacted]	[redacted]	[redacted]	
Batch 43256	[redacted]	[redacted]	[redacted]	

Average content of Myristic acid

g/kg	g/l	% w/w	% v/v
[redacted]	[redacted]	[redacted]	

Section A2.8 Identity of impurities and additives (active substance)

Annex Point IIA2.8

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	*Give date of action*
Materials and methods	*State if the applicants version is acceptable or indicate relevant discrepancies referring to the (sub) heading numbers and to applicant's summary and conclusion.*
Conclusion	*Adopt applicant´s version or include revised version*
Reliability	*Based on the assessment of the method include appropriate reliability indicator*
Acceptability	acceptable / not acceptable *(give reasons if necessary, e.g. if a study is acceptable despite a poor reliability indicator). Discuss the relevance of deficiencies.*
Remarks	
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant´s summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Section A2.10
Annex Point IIA.2.10

Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

Subsection		Official use only
2.10.1 Human exposure towards active substance		
2.10.1.1 Production		
a) Active substance		
i) Description of process	Lauric acid is made in Penang, Malaysia. According to the Guidance on data requirements for active substances and biocidal products (Version 4.3.2 October 2000), no data on the description of the manufacturing process for exposure estimation purpose is necessary.	
ii) Workplace description	See i) Description of process.	
iii) Inhalation exposure	See i) Description of process.	
iv) Dermal exposure	See i) Description of process.	
b) Biocidal product		
i) Description of process	[redacted] Fill the container closure with a suitable filling machine. The preparation takes place at atmospheric pressure.	
ii) Workplace description	The biocidal product is prepared under Good Manufacturing Practices conditions as stipulated for medicinal products.	
iii) Inhalation exposure	Closed machines are used for preparation and the personal wear masks, so there is no probable inhalation exposure during preparation of the biocidal product.	
iv) Dermal exposure	Closed machines are used for preparation and the personal were protective clothes and gloves, so there is no probable dermal exposure during preparation of the biocidal product.	
v) Batch size/throughput	[redacted]	
vi) Shift length	[redacted]	
vii) Frequency of batch per shift	[redacted]	
viii) Throughput per shift	[redacted]	
ix) Days of production	[redacted]	
x) Likely tonnage of the biocidal product to be placed on the market per year	[redacted] depending on the demand of the market.	

Section A2.10
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Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

xi) Form of marketed formulated biocidal product	Lotion in individual bottles with dispenser (one bottle contains [redacted] biocidal product).
xii) Package, storage and transport of the formulated biocidal product	The biocidal product is stored and transported in the package intended for the market (e.g. [redacted]). As package for market e.g. a [redacted] bottle [redacted] with an overcap [redacted] and a pump for easy application is used.
xiii) Workplace description	The formulation of the biocidal product takes places under Good Manufacturing Practices conditions. The machines are closed and the workers are protected with suitable equipment. The cleaning of the machines is done with a validated program by the machines.

2.10.1.2 Intended use(s)

1. Professional/ industrial Users (a.s.)

i) Description of application process	Preparing the biocidal product ContraZeck Lotion gegen Zecken: [redacted] Fill the container closure with a suitable filling machine.
ii) Workplace description	It is worked according to Good Manufacturing Practices. The [redacted] is a closed machine. [redacted] The workers are protected by clothes, gloves, mask and hair cap.
iii) Inhalation exposure	No inhaltive exposure is given, because no temperatures higher than [redacted] °C are used and the components are not volatile exculding the perfume which is added at about room temperature.
iv) Dermal exposure	No dermal exposure of the workers is given, because the manufacturing process is made without dermal contact of the workers who are furthermore protected by clothes, gloves, mask and hair cap.

2. Non-professional Users including the general public (b.p.)

The active substance is used as a lotion for the application on human skin. The preparation is available in a [redacted] container [redacted] Post-application there is no danger of inhalative contact or contact via drinking, food or indirect conctact via environment.

(i) via inhalational contact	The biocidal product is intented for dermal outdoor use and it is rinsed off after use by normal body cleaning. No inhalative contact will take place.

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Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

(ii) via skin contact	The biocidal product is intented for dermal use and it is rinsed off after use. The exposition time of dermal contact is limited. Normaly only a few ml lotion will be used for one application (corresponding to [redacted] lauric acid). At maximum [redacted] the lotion will be applied from one bottle to the human skin. The biocidal product is tested on dermal toxicity [redacted] [130], and [redacted] [20]. The results show that the biocidal product has [redacted].
(iii) via drinking water	The biocidal product is intented for dermal application and it is rinsed off after use. It is not intended for agricultural use which could lead to a contamination of drinking water. Lauric acid as well as the biocidal product is [redacted]
(iv) via food	The biocidal product is intented for dermal application and and it is rinsed off after use. It is not intended for the preparation of food or food ingredients. Nevertheless, lauric acid is constituent of regular human food [56, 59, 61, 121].
(v) indirect via environment	The biocidal product is intented for dermal use and and it is rinsed off after use. It is not intended to be distributed in the environment. Lauric acid as well as the biocidal product are readily biodegradable. Moreover, the quantities, rinsed off during washing process are extremly low [redacted] Considering the natural occurrence of lauric acid the additional quantities reaching sewage are absolutely insignificant.

2.10.2 Environmental exposure towards active substance

2.10.2.1 Production

a) Active Substance

(i) Releases into water	Lauric acid is made in Penang, Malaysia. According to the Guidance on data requirements for active substances and biocidal products (Version 4.3.2 October 2000), no data on the description of the manufacturing process for exposure estimation purpose is needed.
(ii) Releases into air	No release into air is possible, because lauric acid is not volatile.
(iii) Waste disposal	Lauric acid is a solid, waxy substance, which is not soluble in water. In addition, the active substance Lauric acid is readily biodegradable [2] and the waste disposal is insignificant for the intended use as repellent on human skin.

b) Biocidal Product

(i) Releases into water	With a mean yield of [redacted], about [redacted] biocidal product (corresponding to [redacted] lauric acid) will remain in the machine after conclusion of the production process. The machine is cleaned with water at a special temperature. For the validated cleaning process about [redacted] used. So the theoretical concentration of lauric acid in the sewage is [redacted]. This concentration will be further diluted by amounts of sewage in the local sewage plant. The final concentration of the biocidal product is therefore extremly low and will be reduced additionally in the local sewage plant, because the

Section A2.10
Annex Point IIA.2.10

Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

	biocidal product is biodegradable. In addition, fatty acids will reach the sewage in much higher quantities as result of ingestion of regular food and different cleaning processes.
(ii) Releases into air	No release to air is possible, because closed machines are used for the production process.
(iii) Waste disposal	The machines are cleaned with water at a special temperature, no other waste results from the production process.

2.10.2.2 Intended use(s)

Application of the a.s.	The active substance is intended for a preparation of dermal use at human. The active substance will only be used in this preparation.
Application of the b.p.	
	The biocidal product is intended for dermal use at human as a repellent.

a) Active Substance

Affected compartment(s):	The active substance is intended for a preparation of dermal use in humans. The active substance will only be used for the preparation in this biocidal product, so there will be no effected compartiments by the active substance itself.
water	The active substance is intended for a preparation of dermal use in humans. The active substance will only be used in this preparation, so there will be no effected compartiments by the active substance itself.
sediment	The active substance is intended for a preparation of dermal use in humans. The active substance will only be used for the preparation in this biocidal product, so there will be no effected compartiments by the active substance itself.
air	The active substance is intended for a preparation of dermal use in humans. The active substance will only be used for the preparation in this biocidal product, so there will be no effected compartiments by the active substance itself.
soil	The active substance is intended for a preparation of dermal use in humans. The active substance will only be used for the preparation in this biocidal product, so there will be no effected compartiments by the active substance itself.
Predicted concentration in the affected compartment(s):	
water	See b) Biocidal product
sediment	See b) Biocidal product.
air	See b) Biocidal product
soil	See b) Biocidal product

b) Biocidal Product

Affectedcompartment(s):	
water	The biocidal product is intended for dermal use at human. After the outdoor exposure the product is rinsed off with water and soap (containing salts of fatty acids). The concentration in water will be very low by the small amounts of used product and by dilution in the

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Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

effluent system compared to the high amounts of lauric acid, which comes from the regular human food and from the cleaning processes. In addition, lauric acid is readily biodegradable [2] so the compartiment of water is not affected by the intended use.

sediment

The biocidal product is intended for dermal use at human, so no sediment is affected by the product. In addition, the concentration of lauric acid from the biocidal product in the sediment will be extremly low compared to the high amounts of lauric acid, which comes from the regular human food and from the cleaning processes.

air

The physical state of the active substane is solid (melting point [redacted]). The boiling point is very high (about [redacted]) and so the substance is not volatile. So there is no affection of air.

soil

The biocidal product is intended for dermal use at human. No soil is affected by the product.

Predicted concentration in the affected compartment(s)

water

Surface water:

- in the surface water from the [redacted]
  PEC local$_{surface_water}$ = [redacted]
- in the surface water from use [redacted]):
  PEC local $_{surface\_water}$ = [redacted]
- in the surface water from use [redacted]):
  PEC local $_{surface\_water}$ = [redacted]

→ **PEC local$_{surface_water_total}$ =** [redacted]

Sewage treatment:

- in the sewage treatment [redacted]:
  PEC local$_{STP\ water}$ = [redacted]

Ground water:

- in the ground water from the [redacted]
  PEC local$_{ground_water}$ = [redacted]
- in the ground water from use [redacted]):
  PEC local$_{ground\ water}$ = [redacted]

The **PEC local$_{ground\ water}$** from the formulation path is **not** seen as **plausible**, because it results in a higher concentration than in the sewage treatment plant. The sludge from the sewage treatment plant is placed on the fields from where it can reach the ground water which results in a dilution effect. In addition, bringing the sludge from the sewage treatment on the fields will be less probable in the future as it is already prohibited in some European countries or will become prohibited.

In addition, the concentration of lauric acid from the biocidal product in the sewage water will be extremly low compared to the high amounts of lauric acid, which comes from the regular human food and from the cleaning processes.

Because of the ready biodegradability and the small amounts of our product compared to the natural and other sources of lauric acid, the lauric acid from our product will most likely not endanger the ground water.

→ **PEC local$_{ground_water_total}$ =** [redacted]

sediment

- in the sediment from the [redacted]
  PEC local$_{sed}$ = [redacted]
- in the sediment from use [redacted]
  PEC local$_{sed}$ = [redacted]
- in the sediment from use [redacted]
  PEC local$_{sed}$ = [redacted]

→ **PEC local$_{sed_total}$ =** [redacted]

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Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

In addition, the active substance is [redacted] [127], so there will be no detectable concentration over a long time. In addition, the concentration of lauric acid from the biocidal product in the sediment will be extremly low compared to the high amounts of lauric acid, which comes from the regular human food and from the cleaning processes.

air

- in the air from the [redacted]:
  PEC local$_{air}$ = [redacted]
- in the air from use [redacted]
  PEC local$_{air}$ = [redacted]
- in the air from use [redacted]
  PEC local$_{air}$ = [redacted]

→ PEC local$_{air_total}$ = [redacted]

It has to be considered, that the formulation takes place only in a small and restricted place with closed equipment. Therefore the release to air is very restricted and small. And in the sewage treatment a high dilution and biodegradation will take place. Therefore less than calculated from the formulation process will get into the air.
In addition, the biocidal product is not volatile and it is not used as a preparation for fumigants.

soil

- in the soil from the formulation:
  PEC local$_{soil}$ = [redacted]
- in the soil from use ([redacted]):
  PEC local$_{soil}$ = [redacted]

→ PEC local$_{soil_total}$ = [redacted]

It has to be considered, that the formulation takes place only in a small and restricted place. Compared to the PEC local$_{STP\ water}$ the PEC local$_{soil}$ from the formulation is not plausible, because the release on the soil is a further dilution step but the calculated PEC local$_{soil}$ shows a higher concentration than the PEC local$_{STP\ water}$. Therefore PEC local$_{soil_total}$ = PEC local$_{soil}$ from use (body cleaning). In addition, the biocidal product is [redacted] in soil [127], so there will be no detectable concentration over a long time.

Conclusion

For the aquatic environment the PEC/PNEC-ratio is calculated for the

- surface water:
  With the assessment factor [redacted] and
  from the algae study [151] $NOE_rC_{(24\ h)}$ = [redacted]
  → PNEC = [redacted]
  → PEC/PNEC = [redacted] **< 1**
- sewage treatment:
  With the assessment factor (table 17) [redacted]
  from the respiration inhibition test [147] EC50 [redacted]
  → PNEC = [redacted]
  → PEC/PNEC = [redacted] **< 1**
- sediment:
  According to equation no. 70
  → $PNEC_{sed}$ = [redacted]
  → PEC/PNEC= [redacted] **< 1**
- soil:
  According to equation no. 72
  → $PNEC_{sed}$ = [redacted]
  → PEC/PNEC = [redacted]

Section A2.10 Annex Point IIA.2.10	Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

= [redacted] < 1

This PEC/PNEC-ratios show that there is no risk for the environment by the manufacturing and using the biocidal product.
According to the proposed life-cycle of the biocidal product, further calculations of the PEC/PNEC-ratio are not necessary.

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	*Give date of action*
Materials and methods	*State if the applicants version is acceptable or indicate relevant discrepancies referring to the (sub) heading numbers and to applicant's summary and conclusion.*
Conclusion	*Adopt applicant´s version or include revised version*
Reliability	*Based on the assessment of the method include appropriate reliability indicator*
Acceptability	acceptable / not acceptable *(give reasons if necessary, e.g. if a study is acceptable despite a poor reliability indicator). Discuss the relevance of deficiencies.*
Remarks	
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant´s summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Sample table:

Table A2.10: Workplace exposure (biocidal product)

Exposure scenario	Workplace operation	PPE	Year(s) of measurement	Number of measurements	Type of measurements	Exposure concentration
Production	Filling, weighing, mixing	Gloves, clothes, mask, hair cap	No data available*.	No data available*.	personal, closed machine	No data available*.
Formulation	Cleaning	Gloves, clothes, mask, hair cap	No data available*.	No data available*.	personal	No data available*.
Application biocidal product (repellent)	Creaming	No personal protection equipement is necessary.	No data available*.	No data available*.	personal	No data available*.

*No data are necessary, because the biocidal product is easily biodegradable and not harmful to human and nature.

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.1 Melting point, boiling point, relative density (IIA3.1)								
3.1.1 Melting point Melting pt.	Not stated	Purity: [redacted]	**result:** 44 °C [96] **pressure:** no data available.	-	N	2	Product specification from Gustav Heess [1], Gerhartz W. in Ullmann's Encyclopedia of Industrial Chemistry Vol. 10, 5th ed. (1985) 245-276 [96]	
3.1.2 Boiling point Boiling pt.	Not stated	Purity: [redacted]	**result:** 298°C [96] **pressure:** 101.3 kPa	-	N	2	Safety data sheet from Gustav Heess [2], Gerhartz W. in Ullmann's Encyclopedia of Industrial Chemistry Vol. 10, 5th ed. (1985) 245-276 [96]	
3.1.3 Bulk density/ relative density Bulk/rel. density	Not stated	Purity: [redacted]	**result:** d_4^{20}: 0.883 [95]	-	N	2	List of Pharmaceutical Substances,	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
							14th edtion, Prepared and published by ABDATA, Eschborn/ Taunus [3], Bagby MO, in Kirk-Othmer Encyclopedia of Chemical Technology, Vol. 5 (1993) [95]	
3.2 Vapour pressure (IIA3.2)								
Vapour pressure 1	92/69/EEC A.4: Effusion method (Vapour pressure balance), OECD Guideline 104	Purity: [redacted] (w/w) lauric acid, batch no. 43256	**at 25°C:** [redacted]	The pressure was determined in the range between 20°C and 60°C. Above 23°C, a vapour pressure could be measured.	Y	1	Möller, M. Laurinsäure Vapour Pressure A.4, ReportNo. 20070088.01 [139]	
Vapour pressure 2	Baccanari DP et al, The measurement of the vapour pressure, J Phys Chem, 72, 6, 2243-2245, 1968. *C14 labelled lauric acid is used as test substance.*	Purity: not stated	**result:** $2.320 \cdot 10^{-3}$ Pa at 25°C	Vapour pressure of Lauric acid at 25°C is lower than atmospheric pressure. Consequently, evaporation of Lauric acid is extremely low at that temperature.	-	2	Determ Database (see annex 3)	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.2.1 Henry´s Law Constant (Pt. I-A3.2)	Meylan WM, Howard PH, Bond contribution method for estimating Henry´s Law Constants, Environ Toxicol Chem **10**: 1283-1893, published [5]	Purity: not stated	**calculated: result:** $9.31 \cdot 10^{-6}$ atm·m^3/mole at 25°C [6]; **calculated** from the vapour pressure 1 and the water solubility 1 at 25°C: at pH 3: 0.079 Pa*m3/mol at pH 5: 0.041 Pa*m3/mol at pH 7: 0.014 Pa*m3/mol	It is an estimated value from literature, no test is necessary, because the Henry´s law constant is not important for the properties of the biocidal product.	-	2	Record Lauric acid, U.S. National Library of Medicine, Specialized Information System, ChemIDplus [6]	
3.3 Appearance (IIA3.3)								
3.3.1 Physical state	visual assessment	Purity: [redacted] Lauric acid, Batch no. 37077	**result:** [redacted]	GLP is not necessary for the test.	N	1	Testing procedure PA052900 [7], Annex 12	
3.3.2 Colour	visual assessment	Purity: [redacted] Lauric acid, Batch no. 37077	**result:** [redacted]	GLP is not necessary for the test.	N	1	Testing procedure PA052900 [7], Annex 12	
3.3.3 Odour	olfactory assessment	Purity: [redacted] Lauric acid, Batch no. 37077	**result:** [redacted]	GLP is not necessary for the test.	N	1	Testing procedure PA052900 [7], Annex 12	
3.4 Absorption spectra (IIA3.4)								
UV/VIS	Method: Ph. Eur. 5.0, 2.2.25 Absorption Spectrophotometry, Ultraviolet and Visibel	Purity: [redacted] Lauric acid, Batch no. 37077	Batch 37077: See annex 1 and 2: the maximum absorption is at about	-	-	1	Council of Europe [137], Quality Control Dr.	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
	Settings: Range: 200-350 nm Range of Steps: 1 Rate: 50 nm/s Change of bulb: 320 nm		[redacted] nm				R. Pfleger GmbH [138]	
IR 1	[redacted]	Purity: [redacted] Lauric acid, Batch no. 43256	[redacted]	-	Y	1	Roos, M. Characterization of the Molecular Structure of Lauric acid, Report No. B 002/2007 [141]	
IR 2	Range: 4800 – 400 cm^{-1} Solution: 10% CCl_4 for 3800 – 1330 cm^{-1} 10% CS_2 for 1330 – 400 cm^{-1} Sample Preparation: KBr Path length: 0.11 mm Resolution: 2 Sampling procedure: Transmission	Not applicable, because identity and purity are detected by GC.	See annex 4 (Not tested at batch 37077): Principle bands at about 420, 470, 730, 940, 1190, 1230, 1290, 1430, 1470, 1550, 1700, 2680, 2840, 2940 cm^{-1}	-	-	2	NIST webbook (see annex 4)	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
NMR 1	1H-NMR (300 MHz, DMSO-d6, TMS) Sample Preparation: solved in [redacted] containing [redacted] as reference standard Temperature: [redacted] Frequency: [redacted] Relaxation delay: [redacted] Number of scans: [redacted] Equipment: [redacted] 13C-NMR (75.47 MHz, DMSO-d6, TMS): Sample Preparation: solved in [redacted] containing [redacted] as reference standard Temperature: [redacted] Frequency: [redacted] Relaxation delay: [redacted] Number of scans: [redacted] Equipment: [redacted]	Purity: [redacted] lauric acid, Batch no. 43256	See Literature Reference 141 Roos M. ^{1}H-NMR: δ = [redacted] ^{14}C-NMR: δ = [redacted]	-	Y	1	Roos, M. Characterization of the Molecular Structure of Lauric acid, Report No. B 002/2007 [141]	
NMR 2	Solvent: Chloroform-D Apparat: Brücker AC 200 Frequency: 50 MHz Evaluation: shifts as units relative to tetramethylsilane as internal standard.	Not applicable, because identity and purity are detected by GC.	See annex 5 (Not tested at batch 37077): Majour chemical shifts at: 180 ppm, 34 ppm	-	-	2	Dimas DA et al [93]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
MS 1 (GC-MS)	MS (TIC-Detector) Sample Preparation: solved in [redacted] Equipment: [redacted]	Purity: [redacted] lauric acid, Batch no. 43256	In accordance with the structure with m/z = [redacted]	-	Y	1	Roos, M. Characterization of the Molecular Structure of Lauric acid, Report No. B 002/2007 [141]	
MS 2	Owner: NIST Mass Spectrometry Data Center Origin: Chemical Concepts Intrument IE (eV) 70 EPA MS number 221043	Not applicable, because identity and purity are detected by GC.	See annex 6 (Not tested at batch 37077): Major ions at about m/z 30, 40, 55, 70, 85, 95, 110, 115, 130, 140, 155, 172, 200	-	-	2	NIST webbook (see annex 6)	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.5 Solubility in water (IIA3.5) Water solubility 1	92/69/EEC, A.6 (flask method), OECD Guideline 105	Purity: [redacted] lauric acid, Batch no. 43256	**results:** [redacted] L at [redacted] °C; [redacted] L at [redacted] °C; [redacted] L at [redacted] °C **temperature:** [redacted] °C; [redacted] °C; [redacted] °C **pH:** [redacted] --- **results:** [redacted] L at [redacted] °C; [redacted] L at [redacted] °C; [redacted] L at [redacted] °C **temperature:** [redacted] °C; [redacted] °C; [redacted] °C **pH:** [redacted] --- **results:** [redacted] L at [redacted] °C; [redacted] L at [redacted] °C; [redacted] L at [redacted] °C **temperature:** [redacted] °C; [redacted] °C; [redacted] °C **pH:** [redacted] --- [redacted] (T = 20 °C, pH = [redacted])	The water solubility was determined in dependence of pH and temperature. [redacted] is determined for the test item lauric acid. The solubilities of lauric acid at pH [redacted] and pH [redacted] show [redacted] During the course of the study [redacted].	Y	1	J. Lange, Lauric acid Water Solubility in Dependence of pH and Temperature (Flask Method), Project-N. 061207PG [142]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
				[redacted] pH = [redacted]) and furthermore [redacted] (e.g. [redacted]). The test item showed a typical solubility profile.				

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
Water solubility 2	Conductometric Titration with $Ba(OH)_2$ [98], [99]	Purity: not stated	**result:** 5.5 mg/ 100 g water **temperature:** 20 °C **pH:** -	Carbon dioxide was taken into account in the method of analysis [102].	-	1	Lide DR (ed.) [94], Bagby MO [95], Brockmann R et al [96], Fasman GD [97], Ralston AW, Hoerr CW [98], Ralston AW et al [99], Singleton WS [100]	
Water solubility 3	Film balance: measuring of the π-A curve [101] Conductivity, Grinnell Jones-Dyke type of bridge supplied by Leeds and Northrup [102]	Purity: not stated	**result:** 0.42 mg/100 ml water at 25°C [101] 0.48 mg/100 ml water at 25°C [102] **temperature:** 25°C (and 50°C [102]) **pH:** 5.7 [101]	The disagreement between the data of Lide DR/Bagby MO/Brockmann R/Fasman GD/ Ralston and Robb/John is possibly due to the different amounts of ionized species present [101].	-	1	Robb ID [101] John LM et al [102]	
3.6 Dissociation constant (-)	Serjeant EP, Dempsey B, Ionization Constants of Organic Acids in Aqueous Solution, Pergamon, Oxford, 1979, published [8, 149]: Measurement of pH changes during titration of Na-salt below c.m.c	Purity: not stated	5.3 at 20°C	An experimental value from literature is sufficient and adequate.	-	2	U.S. National Library of Medicine, Specialized Information System, ChemIDplus [6], Nyren V, Back E [149]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.7 Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)	Inspection of literature	Purity: not stated	**result:** soluble in ethanol and propanol, very soluble in benzene and ether.	No test is necessary because the solubility in organic solvents is not important for the intended use.	-	1	List of Pharmaceutical Substances, 14th edtion, Prepared and published by ABDATA, Eschborn/ Taunus [3]	
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)	M1000001 (appearance) M1000034 (odour)	Purity: [redacted] lauric acid Specification: [redacted]	**result (Batch 37077):** [redacted]	[redacted]	N	1	Testing procedure PA701550, Stability Data [91]	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.9 Partition coefficient n-octanol/water (IIA3.6)								
log Pow 1:	92/69/EEC, A.8 (HPLC-Method), OECD Guideline 104	Purity: [redacted] lauric acid, Batch no. 43256	**result:** log Pow = [redacted] (pH = [redacted]) log Pow = [redacted] (pH = [redacted]) log Pow = [redacted] (pH = [redacted]) **temperature:** [redacted] **pH:** [redacted]	According to the guidelines EC A.8 and OECD 104 the test should be conducted [redacted] Only one temperature was tested, [redacted]	Y	1	J. Lange, Lauric acid Partition Coefficient (n-octanol/water) using HPLC-Method, projectNo. 061207PG [143]	
log Pow 2:	Inspection of a manufacturer's data sheet.	Purity: not stated	**result:** Log p(o/w) 4.2 **temperature:** no data available **pH:** no data available	No test is necessary because the log Pow is not important for the intended use.	N	1	Safety data sheet from Merck [4]	
3.10 Thermal stability, identity of relevant breakdown products (IIA3.7) Thermal stability 1	CIPAC MT 46.1/46.2/46.3 OECD Guideline 113	Purity: [redacted] lauric acid, Batch no. 48290	**result:** [redacted] were detected → [redacted] **temperature:** [redacted]	GLP is not necessary for the accelerated storage test.	N	1	Kohles T [156, 157]	
Thermal stability 2	Identification of relevant breakdown	The main degradation	**result:** Possible breakdown	GLP is not necessary for the test.	N	1	Brockmann R et al [96],	