GreenScreen® Chemical Assessment

[Heptyl Glucoside (100231-64-9)]

Method Version: GreenScreen® Version 1.4

Assessment Details:

Assessment Type[1]:	Certified
Assessment Prepared By:	WAP Sustainability, LLC
Assessment Prepared For:	WA Department of Ecology
Date Assessment Completed:	7/3/2023
Assessment Expiration Date:	7/3/2026
Assessor Type: (Licensed GreenScreen Profiler or equivalent, Authorized GreenScreen Practitioner or Unaccredited)	Licensed GreenScreen® Profiler

[1] **Assessment Type**: GreenScreen reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen Practitioner), or "CERTIFIED" (by Licensed GreenScreen Profiler or equivalent)

GREENSCREEN BENCHMARK™ SUMMARY:

This chemical assessment report includes a GreenScreen Benchmark™ score and results for Heptyl Glucoside (100231-64-9)] only.

No marketing claims can be made without licensing through Clean Production Action.

GreenScreen Benchmark Score:
Heptyl Glucoside (100231-64-9)] was assigned a Benchmark Score of U as the chemical does not meet the minimum data requirements for Benchmark-2. Specifically, a data gap exists for carcinogenicity. In a worst-case scenario, if Heptyl Glucoside were assigned a high score for carcinogenicity activity it would be assigned a score of Benchmark 1.

HAZARD CLASSIFICATION SUMMARY

Table 1. GreenScreen Hazard Summary Table:

GreenScreen Hazard Summary Table for Heptyl Glucoside (100231-64-9)																			
Group I Human					**Group II and II* Human**									**Ecotox**		**Fate**		**Physical**	
Carcinogenicity	**Genotoxicity/Mutagenicity**	**Reproductive Toxicity**	**Developmental Toxicity**	**Endocrine Activity**	**Acute Toxicity**	**Systemic Toxicity**		**Neurotoxicity**		**Skin Sensitization***	**Respiratory Sensitization***	**Skin Irritation**	**Eye Irritation**	**Acute Aquatic Toxicity**	**Chronic Aquatic Toxicity**	**Persistence**	**Bioaccumulation**	**Reactivity**	**Flammability**
						single	repeat*	single	repeat*	*	*								
DG	L	*M*	**L**	DG	**L**	**L**	*L*	*M*	DG	**L**	DG	*H*	*vH*	**L**	**M**	**vL**	**vL**	*L*	**L**

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. Group II Human Health endpoints differ from Group II* Human Health endpoints in that Group II Human Health endpoints have four hazard scores (i.e., vH, H, M and L) instead of three (i.e., H, M and L), and are based on single exposures instead of repeated exposures. Group II* Human Health endpoints are indicated by an * after the name of the hazard endpoint or after "repeat" for repeated exposure sub-endpoints.

SCOPE OF ASSESSMENT

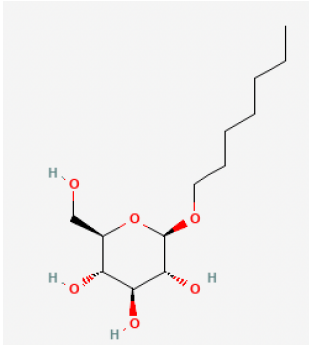
Chemical Name (CASRN): Heptyl Glucoside (100231-64-9)

Also Called (List Synonyms):

Pubchem 2023
Heptyl D-glucoside
EINECS 309-364-8
100231-64-9
CHEMBL1170455
C13-H26-O6
Heptyl hexopyranoside
n-Heptyl ?-D-glucopyranoside
SCHEMBL14210465
SCHEMBL22111992
DTXSID90905277
BDBM50347460

Chemical Structure:

PubChem 2023



Suitable analogs or moieties of chemicals used in this assessment (CASRN(s)):

ECHA 2023b

Structural similarities of the category substances are reflected in similar physico-chemical properties and mode of action. Alkyl polyglycosides have a common metabolic fate that involves hydrolysis of the alpha- and beta-glycosidic bond to the fatty alcohol and glucose. Glucose and glucose oligomers enter the carbohydrate metabolic pathway and are catabolised into pyruvate and subsequently to the major extent into acetyl-CoA, which is introduced into the citric acid cycle with the aim to generate reduction equivalents for energy generation in the oxidative phosphorylation. Fatty alcohols, representing the main difference in the structure of different alkyl polyglycosides, are oxidized to the corresponding fatty acid and fed into the physiological pathway of beta-oxidation, where they are also oxidised to

acetyl-CoA. In addition to its function in the generation of energy by catabolic processes acetyl-CoA can also be used in anabolic processes like lipid synthesis, which is important for the storage of energy in form of large high-energy macromolecules. There is convincing evidence that these chemicals lie in the overall common profile of this category or sub-category, respectively. The key points that the members share are:

(i) Common origin: produced from fatty alcohols, reacting with D-glucose in the presence of an acid catalyst.

(ii) Similar structural features: aliphatic hydrocarbon chain bound to glucose oligomers by alpha or beta glycosidic bond.

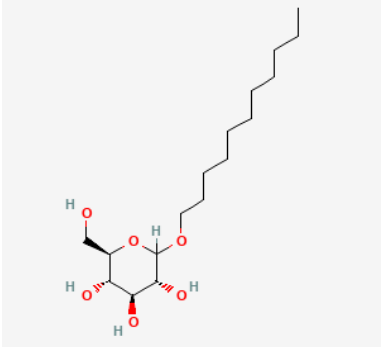
(iii) Similar physico-chemical properties: trend in log Pow based on alkyl chain length and degree of glycosylation; low vapour pressure; water solubility decreasing with the alkyl chain length, starting from very high and high values up to insoluble C16-18; surface active substances fully dissociated in water (exception: C16-18).

(iv) Common properties for environmental fate & eco-toxicological profile: readily biodegradable, no potential for bioaccumulation, low to moderate adsorption potential, clear trend in aquatic toxicity (increasing toxicity with increasing carbon chain with a maximum at C12-16 and then decreasing), no potential for sediment and soil toxicity.

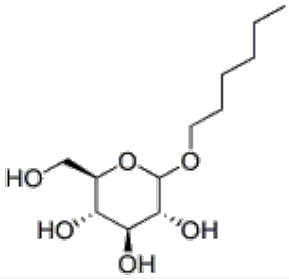
(v) Similar metabolic pathways: absorption in the intestine, hydrolysis of the alpha- and beta-glycosidic bond in intestine and further metabolism of the breakdown products sugar and alcohol. Alkyl polyglycosides with alpha-glycosidic bond may already be hydrolysed in the saliva by enzymatic activity of alpha-amylases.

(vi) Common levels and mode of human health related effects: skin and eye irritating properties of the alkyl polyglycosides represent the main factor for effects on human health. The similar toxicokinetic behaviour (hydrolysis of the alpha- and beta-glycosidic bonds) results in structural similar cleavage products, which show a low toxicity after acute and repeated oral exposure. Furthermore, all category members are not sensitising, not mutagenic or clastogenic, and have shown no reproduction and developmental toxicity.

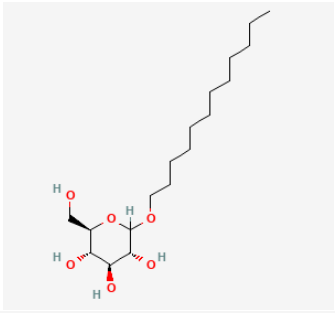
Chemical Structure(s) of suitable analog(s) and/or moieties:



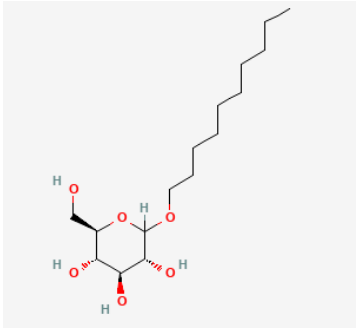
Undecyl glucoside (CAS# 98283-67-1)



Hexyl D-glucoside (CAS# 54549-24-5)



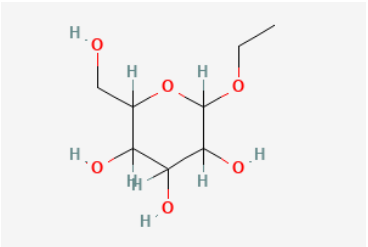
Lauryl glucoside/ D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS#)110615-47-9



Capryl glycoside/ Decyl glucoside (CAS# 68515-73-1)

No Structure Available

C8-10-alkyl glycosides (no CAS# or structure available)



Ethyl glucoside (CAS# 3198-49-0)

Identify potential applications/functional uses of the chemical:

PubChem 2023
1. Body cleaners containing abrasives or exfoliants
2. Rinse-out everyday hair conditioners (excluding combo shampoo/conditioner products)
3. Leave-in everyday hair conditioners and detanglers
4. Shampoos, including dual shampoo/conditioner products

Table 2. Environmental Transformation Products Summary

Life Cycle Stage	Transformation Pathway	Environmental Transformation Product	CAS #	Feasible (Yes or No)	Relevant (Yes or No)	GreenScreen List Translator Score or GreenScreen Benchmark Score
End of life	Central cleavage	Glucose	50-99-7	Y	N	BM-3
End of life	Central cleavage	Heptanoic acid	111-14-8	Y	Y	LT-UNK

The biodegradation pathway of alkyl polyglycosides has not been elucidated. Polyglycoside alkanoic acids, possible intermediates of ω- and β-oxidation of the alkyl chain, were not detected during degradation of alkyl polyglycosides in a fixed-bed reactor. Based on this finding, Eichhorn et al. hypothesized that alkyl polyglycosides are degraded through a central cleavage. Central cleavage results in the formation of saccharides and fatty acids (C.G. van Ginkel 2007). This would result in primary degradation products of glucose and heptanoic acid. Glucose is a substance necessary for life or commonly formed in the ambient environment and therefore is not considered relevant. Both heptanoic acid and glucose released from primary degradation are not likely to persist in the environment, and thus do not affect the benchmark score for heptyl glucoside.

HAZARD CLASSIFICATION SUMMARY[2,3]

GROUP I HUMAN HEALTH EFFECTS (GROUP I HUMAN)

Carcinogenicity (C): DG

Heptyl Glucoside was assigned a hazard classification level of Data Gap for carcinogenicity. No data was located for the compound of interest or analog compounds that addressed the carcinogenicity endpoints.

Data
- Lists
  - *Authoritative: None*

[2] Include computer-modeling outputs in Appendix C.
[3] References may be provided under each hazard endpoint or at the end of document.

    - *Screening: None*
- Measured Data: None
- Estimated Data: None

Mutagenicity/Genotoxicity (M): L

Heptyl Glucoside was assigned a hazard classification level of Low for Mutagenicity/Genotoxicity based on negative in vitro assays and all in vivo results reported for the compound of interest. This low score is supported by negative results reported for analog compounds. The low hazard conclusion is based on high quality studies reported for the chemical of interest therefore reported with high confidence.

Data

- Lists
    - *Authoritative: None*
    - *Screening: None*
- Measured Data

NICNAS 2015

- OECD TG 471 Bacterial Reverse Mutation Test: In the dose finding tests and the main tests, increases in the number of revertant colonies or a dose-related response was not observed for any dose with or without metabolic activation. The notified chemical was not mutagenic to bacteria under the conditions of the test.
- OECD TG 474 Mammalian Erythrocyte Micronucleus Test: Premature death occurred at and above 500 mg/kg, clinical signs were observed at and above 250 mg/kg including hunched posture, lethargy, pilo-erection, decreased respiratory rate, ptosis, ataxia, splayed gait, prostration, labored respiration, and pallor of the extremities. There was a statistically significant increase in the incidence of micronucleated polychromatic erythrocytes in the mid-dose group but was within the historical range for vehicle controls. There was a statistically significant decrease in the PCE/NCE ratio in the 24 h high dose group. The response was considered part of a dose related effect indicating exposure of the bone marrow to the test material. The test material was considered to be non-genotoxic under the condition of the test.

ECHA 2023a

- The bacterial mutagenicity of alcohol polyglycosides (APGs) was examined with hexyl-D-glucoside, branched and linear C9-11-alkyl glycosides and C10-16-alkyl glycosides using several strains of S. typhimurium or E. coli. All tests were conducted according or similar to OECD Guideline 471 in the presence and absence of metabolic activation. The results revealed that APG can be considered as non-mutagenic.
- The clastogenic potential of APG in vitro was analyzed by a chromosome aberration test according to OECD 473 in Chinese Hamster lung fibroblasts with C10-16-alkyl glycosides. No chromosomal aberrations (ABs) were induced in the presence and absence of metabolic activation and therefore, APG are considered to be non-clastogenic in vitro.

- Testing of the mammalian mutagenicity in vitro was done by a Mouse Lymphoma Assay with C8-10-alkyl glycosides and had a clear negative outcome, hence it can be concluded that APG are not mutagenic in mammalian cells.
- The clastogenic potential was additionally tested in vivo by a murine micronucleus assay which indicated as well a negative result.

- Estimated Data: None

Reproductive Toxicity (R): *M*

Heptyl Glucoside was assigned a hazard classification level of Moderate for Reproductive Toxicity based on reported effects on testes in rabbits following dermal exposures to the analog caprylyl/capryl glucoside . It is unclear if these effects are directly related to exposure or were secondary effects caused by the stress related to the exposure method. The reported testicular effects following dermal exposures is not sufficiently convincing to assign a category 1 GHS classification for the compound. In addition, following OECD guideline 421, no adverse effects were observed in male and female rat reproductive organs at the highest Hexyl D-glucoside dose of 1000 mg/kg bw/day. Similarly, no clinical signs and no effects on body weight, food consumption, estrous cycle and sperm parameters were recorded for parental animals orally exposed to D-Glucopyranose, oligomeric, C10-16-alkyl glycosides. In addition, exposures to lauryl glucoside produced no test article related effects on reproductive parameters. The hazard conclusion is conservatively based on equivocal evidence for testicular effects and is therefore reported as low confidence.

Data
- Lists
    - *Authoritative: None*
    - *Screening: None*
- Measured Data

ECHA 2023a

- In a one-generation screening assay according to OECD 421, the test substance (APG C12–C14 fatty alcohol from renewable sources, n = 1.43) was applied to 40 males and 40 females Sprague-Dawley rats prior to mating, throughout the gestation and lactation period until postpartum day 3. Treatment by gavage with 0, 100, 300 and 1000 mg/kg bw/day began 7 days after allocation for both males and females. Treatment commenced when males and females were approximately 12 weeks of age, 2 weeks before pairing and continuously thereafter, up to the day before sacrifice (study day 53, day 4 postpartum). Matings were monogamous. During the study, parameters of general toxicity like clinical signs, food consumption and body weight gain were recorded in the parental generation and in the pups. Effects related to reproduction and hormone balance such as estrous cycle, mating performance, pregnancy rates and the number of embryo resorptions were registered. Pup losses were recorded, and the filial generation was examined for behavioral abnormalities and external growth abnormalities. No effects on the fertility were observed up to the highest dose of 1000 mg/kg bw/day.

Under the conditions of a state-of-the-art reproduction/developmental toxicity screening testing according to the OECD guideline 421, no adverse effects were observed regarding male and female reproductive organs even at the very high dose of 1000 mg/kg bw/day. The lack of major toxicity was further confirmed by a sub-chronic toxicity study in Sprague–Dawley rats that did not show any substance related systemic toxic effects in either gender up to the limit dose of 1000 mg/kg bw (Potokar et al., 1989).

ECHA 2023b

- A key reproduction/developmental toxicity screening test performed according to OECD TG 421 with the category member D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9) is available (Messinger et al., 2007). Groups of 10 Sprague-Dawley rats of each sex per dose were administered doses of 100, 300 and 1000 mg/kg bw/day via oral gavage. Males were treated for at least 4 weeks on 7 consecutive days per week, starting from 2 weeks prior to mating; females were treated for 2 weeks prior to mating, during mating and gestation on 7 consecutive days per week until day 4 post-partum. The animals were monitored for clinical signs, body weight, food consumption, mating, and litter performance, estrous cyclicity and sperm parameters. All animals were submitted to necropsy, which included weighing of testes and epididymites. No information on histopathological examination is available. Gross pathology was performed with all parental animals and the offspring. No clinical signs and no effects on body weight, food consumption, estrous cycle and sperm parameters were recorded for parental animals during the entire study period. In males and females, no substance-related effects on fertility index were observed. A slight, but not significant decrease in copulatory index was observed in females receiving the high dose (1000 mg/kg bw/day). One female in the mid-dose group and two females in the high-dose group did not mate until day 10 and were mated with another male afterwards. One female in the high dose group did not mate after a period of 20 days. No effects on relative and absolute weights of testis, epididymis, and seminal vesicles were observed between test substance-treated and control animals. A marginal reduction in absolute and relative prostate weights in all treated males compared to the control group was noted. In the low dose group (100 mg/kg bw/day) a significant reduction in the weights of prostate were observed. Due to the absence of dose-dependency, this effect was not considered to be biologically significant. Gross pathology revealed no substance-related effects for parental animals. No effects on mean litter weights and sex ratios were observed between the F1 generations of treated and control animals. Some slight, but not significant variations in pre-birth loss were seen in the high-dose group compared to controls. Based on the results of the study and due to the absence of any toxicologically relevant adverse effect a NOAEL of 1000 mg/kg bw/day was derived for systemic and reproductive toxicity.

CIR 2011

- Lauryl glucoside (as APG C12-C14 fatty alcohol from renewable sources, n: 1.43) was given orally, by gavage, to groups of 10 male and 10 female Sprague-Dawley rats at doses of 0, 0.1, 0.3, or 1 g/kg/day, from 2 weeks prior to mating to 4 days after delivery. No signs of general toxicity were observed in the parental animals. The relative and absolute weights of the testes, epididymides, and seminal vesicles were similar for

treated and control animals. There were no test article related effects on reproductive parameters. The mean litter weights, mean pup weights, sex ratio, and gestation period was similar for all groups; a slight variation in pre-birth loss observed in the high-dose group was not statistically significant.

- Groups of 6 male and 6 female NZW rabbits were dosed dermally with 0, 0.9, and 1.8 g ai/kg (0, 22.5, and 45 w/v%, respectively) caprylyl/capryl glucoside (60% active CAS# 68515-73-1) in distilled water (4 mL/kg). Ten 6-hour occlusive applications were made over a 2-week period. Treatment-related signs of toxicity, such as ataxia, lethargy, and emaciation, were observed in both the test groups. One female of the 1.8 g ai/kg group died after 10 doses, and the death was considered test article related. Slight irritation was observed 1 day after the initial dose, and severe dermal irritation was observed in males and females of both the test groups by days 5 to 6 of the study. Body weights of treated male and female rabbits were significantly less than those of the controls, and mean bw loss was observed for both the groups. Compared to the controls, absolute testes weights were significantly lower in treated males of both the dose groups. No other compound-related changes in organ weights were observed. Small testes were observed in 3 of the 6 treated males of each group; the researchers stated that occurrence of this lesion was rare, and while the occurrence was not statistically significantly different from controls, it was considered biologically significant. Microscopic examination of selected male tissues demonstrated very slight to marked testicular degeneration in all rabbits in the 0.9 g ai/kg group and slight to marked testicular degeneration in 4 rabbits of the 1.8 g ai/kg group. Very slight to moderate atrophy of the prostate and “accessory sex glands” was observed in 3 rabbits of each group. The researchers stated that irritation, inflammation, and stress in these animals were major contributing factors to many, if not all, of the toxicologic effects; however, the researchers also stated that it is possible that caprylyl/capryl glucoside produced some of the effects. (Published findings have reported that degenerative changes occur commonly in the testes of normal rabbits, and these changes may be increased during stress. A No-Observed-Effect Level (NOEL) was not obtained.
- In a 2-week study, 10 occlusive applications of 0.14, 0.41, and 1.25 g ai/kg (60% active) caprylyl/capryl glucoside in distilled water (0, 3.5, 10.4, and 31.1% ai, respectively) were made to intact skin on the backs of 6 male NZW rabbits per group in order to determine the NOEL for testicular toxicity. Two of the high-dose animals died during the study, and the 4 surviving animals had signs of treatment-related toxicity. No treatment-related mortality occurred in the low- or mid-dose groups. Dermal irritation, which progressed from slight to severe with time, was observed in all test groups, and slight to moderate irritation was observed in the controls. Changes in some hematology and clinical chemistry values were observed but were attributed to stress of the occlusive procedure, irritation, and bw loss. A decrease in the mean absolute testicular weights in animals of the mid- and high-dose groups was considered treatment related. A treatment-related loss in bw was observed in all the test groups, and the mean terminal bws of rabbits of all test groups were decreased compared to controls. Relatively small testes were observed in 1, 2, 4, and all 6 males of the control, low-, mid-, and high-dose groups, respectively. Treatment-related microscopic changes were observed in the testes, epididymides, prostate, and vesicular glands of the mid- and high-dose group animals; some of the lesions included an increased incidence and severity of diffuse bilateral testicular atrophy with necrotic spermatocytes and atrophy of the prostate and vesicular glands. The NOEL for the microscopic effects in the epididymides, prostate, and

vesicular gland was 0.14 g ai/kg. One rabbit of the low-dose group, which had the greatest bw loss, had moderate testicular atrophy and a moderate number of necrotic spermatocytes/spermatids. The researchers stated that the testes and accessory sex organs of the animals in the control and treatment groups were relatively immature due to age (12 weeks) and low bws, and the immature nature of these organs complicated the evaluation. Changes in the testes and accessory sex glands were attributed to the stress. A NOEL for the study was not established.

- In yet another 2-week study, using nonocclusive applications, 2 mL of 0, 0.06, 0.18, or 0.54 g ai/kg caprylyl/capryl glucoside (60% active) in distilled water (corresponding to concentrations of 0, 3, 9, and 27% ai, respectively) were applied to the intact skin of the backs of 6 male rabbits/group. These doses were selected following a 2-week pilot study, in which unoccluded exposure to 0.12, 0.23, and 0.45 ai g/kg caprylyl/capryl glucoside produced slight to moderate erythema and edema. In the main study, treatment-related signs of toxicity were not observed. Slight dermal irritation was observed in all the groups after the initiation of dosing; the irritation became moderate in the high-dose group after 3 days of dosing. Body weights of rabbits of the high-dose group were slightly, but significantly, decreased compared to controls. Absolute testes weights were slightly, but not significantly, decreased in the high-dose group. No treatment-related effects on hematology or clinical chemistry values or organ weights were reported. Microscopically, epithelial hyperplasia, hyperkeratosis, congestion, and eschar formation were observed in the skin of rabbits of the high-dose group; these changes were not observed in rabbits of the other test groups. No test article-related microscopic changes were observed in the testes or accessory sex glands at any dose. The NOEL for systemic toxicity was 0.18 g ai/kg caprylyl/capryl glucoside.

- Estimated Data: None

Developmental Toxicity incl. Developmental Neurotoxicity (D): L

Heptyl Glucoside was assigned a hazard classification level of Low for developmental toxicity based on available study data in analog compounds. Specifically, following OECD guideline 414, no adverse developmental effects were observed in male and female rat fetuses at the highest Alkyl glucoside (C10–14, n = 1.4) dose of 1000 mg/kg bw/day. Similarly, a prenatal developmental toxicity study performed with D-Glucopyranose, oligomeric, C10-16-alkyl glycosides according to OECD 414 and in compliance with GLP did not reveal any treatment-related effect. In addition, exposures to lauryl glucoside produced no statistically significant article related effects on developmental endpoints. The hazard conclusion is based on guideline studies using high quality analogs and is therefore reported as high confidence.

Data

- Lists
  - *Authoritative: None*
  - *Screening: None*
- Measured Data

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- Alkyl glucoside (C10–14, n = 1.4) was tested according to OECD 414 at dose levels of 0, 100, 300 and 1000 mg/kg bw/day in 96 female Sprague-Dawley rats. The test substance was administered orally by gavage once daily from day 6 to day 15 of gestation. Control animals receive the vehicle alone (aqua dest.) for the entire test period. Clinical conditions and reactions to treatment were recorded at least once daily. Body weights were reported for days 0, 6, 16 and 20 of gestation. All surviving females were sacrificed on day 20 of gestation and the fetuses were removed by caesarean section. At necropsy, the females were examined macroscopically, and live fetuses were weighted, sexed, and examined for visceral and skeletal abnormalities. Gross macroscopic examinations include all maternal organs with emphasis on the uterus, uterine contents, position of fetuses in the uterus and number of corpora lutea. Number and distribution of intrauterine implantations were classified as live or dead fetuses, late intrauterine deaths (resorptions), early intrauterine deaths (resorption sites). The fetuses were removed from the uterus, were sexed, weighted individually, and examined for gross external abnormalities and placentae were weighted separately. The brains and viscera of half of the fetuses of each litter were examined as well as skeletal abnormalities in the other half of the litter. Skeletal and visceral investigations did not detect any treatment-related malformations. For the embryo/fetotoxicity, the teratogenicity and the maternal toxicity a NOAEL of 1000 mg/kg was deduced.

ECHA 2023b

- A prenatal developmental toxicity study performed with D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS# 110615-47-9) according to OECD 414 and in compliance with GLP with the test material and did not reveal any treatment-related effect. Thus, a NOAEL (maternal/developmental) of ≥1000 mg/kg bw/day was derived. The test substance was only administered during organogenesis and not through the entire period of gestation to the day before caesarean section; body weights were not determined in 3-day intervals during treatment period.

CIR 2011

- Lauryl glucoside (as APG C12-C14 fatty alcohol from renewable sources, n: 1.43) was given orally, by gavage, to groups of 10 male and 10 female Sprague-Dawley rats at doses of 0, 0.1, 0.3, or 1 g/kg/day, from 2 weeks prior to mating to 4 days after delivery. No signs of general toxicity were observed in the parental animals. The mean litter weights, mean pup weights, sex ratio, and gestation period was similar for all groups; a slight variation in pre-birth loss observed in the high-dose group was not statistically significant.

- Estimated Data: None

Endocrine Activity (E): DG

Heptyl Glucoside was assigned a hazard classification level of Data Gap for Endocrine Activity based on lack of adequate studies. While one study reporting negative findings in the E-Screen assay using the analog lauryl glucoside, this single study does not provide sufficient evidence to suggest the absence of endocrine activity is associated

with the chemical. No additional data was located for any of the compound of interest of analogs of the compound.

Data
- Lists
  - *Authoritative: None*
  - *Screening: None*
- Measured Data

CIR 2011

- Lauryl glucoside (as APG C12-C14 fatty alcohol from renewable sources, n: 1.43) was evaluated in the E-Screen assay, in which the induction of cell proliferation in the estrogen-dependent human breast tumor MCF-7 cells is determined, at concentrations of 0.1-10,000 nmol/ml. 17-β-Estradiol and bisphenol-A were reference substances, and the medium was the negative control. No effects were reported at concentrations up to 105 higher than the concurrent controls. The effects of 0.1-1000 nmol/ml lauryl glucoside (as APG C12-C14 fatty alcohol from renewable sources, n: 1.43) were determined in the MCF-7 reporter gene assay, in which the induction of luciferase activity in stable transfected MCF-7 cells is determined. No effects were seen with lauryl glucoside alone, and no anti-estrogenic or other synergistic effects were observed after incubation with 0.01-1000 nmol/ml estradiol:lauryl glucoside (1:1 molar ratio).

- Estimated Data: None

GROUP II AND II* HUMAN HEALTH EFFECTS (GROUP II AND II* HUMAN)

Note: Group II and Group II endpoints are distinguished in the v1.4 Benchmark system (the asterisk indicates repeated exposure). For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints. See GreenScreen Guidance v1.4, Annex 2 for more details.*

Acute Mammalian Toxicity (AT): L

Heptyl Glucoside was assigned a hazard classification level of Low for acute mammalian toxicity based on oral and dermal study data for the compound of interest. This hazard conclusion is supported in numerous studies using analogs which report LD50 values >2000 mg/kg bw for both oral and dermal exposures pathways. No inhalation data was located however the low volatility of the substance (i.e., vapor pressure of 7.2×10^{-8} kPa at 20 °C) indicates that inhalation exposures are not a significant pathway of exposure. The hazard score is based on guideline studies using high quality analogs and is therefore reported as high confidence.

Data
- Lists
  - *Authoritative: None*

    - *Screening: None*
- Measured Data

NICNAS 2015

- OECD TG 423 Acute Oral Toxicity – Acute Toxic Class Method and test method B.1 tris of Council regulation No. 440/2008. reports LD50 >2000 mg/kg bw for female rats
- In anOECD TG 402 Acute Dermal Toxicity reports LD50 >2000 mg/kg bw for male and female rats

ECHA 2023a

- The oral LD50 values, tested with C8-10-alkyl glycosides and C10-16-alkyl glycosides were both above 2 g/kg. The same result was achieved for the dermal route when tested with C8-10-alkyl glycosides and C10-16-alkyl glycosides.

ECHA 2023b

- In this key acute oral toxicity study following the acute toxic class method (OECD TG 423, GLP) six female fasted Sprague Dawley rats were administered a single dose of 2000 mg/kg bw of the test substance D-Glucopyranose, oligomeric, undecyl glycoside whereas another six females (control animals) received the vehicle alone (distilled water) in a stepwise procedure (three rats per step) via oral gavage (Phycher Bio Development, 2008). The acute oral LD50 value for females was considered to be greater than 2000 mg/kg bw.
- A reliable key acute dermal toxicity study performed equivalent or similar to OECD TG 402 and in compliance with GLP with the category member D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9) is available (Hill Top Biolabs, 1989). In this limit test five New Zealand White rabbits of each sex were exposed to a single dose of 2000 mg/kg bw of the test substance for 24 h via semi-occlusive dressing and observed for 14 days post-application. The acute dermal LD50 value was calculated to be greater than 2000 mg/kg bw.
- A reliable supporting acute dermal toxicity study performed equivalent or similar to OECD TG 402 and in compliance with GLP with the category member D-Glucopyranose, oligomers, decyl octyl glycosides (CAS 68515-73-1) is available (Hill Top Research, 1987). In this limit test five New Zealand White rabbits of each sex were exposed to a single dose of 2000 mg/kg bw of the test substance for 24 h via semi-occlusive dressing and observed for 14 days post-application. The acute dermal LD50 value was calculated to be greater than 2000 mg/kg bw. One animal died during the 14-day observation period (Day 13).

CIR 2011

- C10-16 Alkyl Glucoside Groups of 5 male and 5 female NZW rabbits were given a single dermal dose of g/kg bw C10-16 alkyl glucoside, 50% a.i. (as C10-16 APG; n:1.6). (Whether occlusion was used was not stated.) None of the animals died during the study.
- Female NMRI mice were given a single oral dose of 0.040 g (2 g/kg bw) caprylyl glucoside as a suspension in 0.2 ml of a 5% aq. solution of phosphatidylcholine. No

toxic effects were observed during a 2-wk post-dose observation period.
- Groups of 5 male and 5 female Sprague-Dawley rats were given a single oral dose of 5 g/kg bw caprylyl/capryl glucoside (as C8/10 APG; n:1.6, 50% a.i.). None of the animals died during the study.
- Groups of 5 male and 5 female Sprague-Dawley rats were given a single oral dose of 5 g/kg bw C10-16 alkyl glucoside (as C10/16 APG; n:1.6, 50% a.i.).20 None of the animals died during the study. Additionally, no mortality was observed upon dosing of 2 male and 2 female Wistar rats with a single oral dose of 2 g/kg bw C12/14 APG, n: 1.6 and 60% a.i.

- Estimated data: None

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST-single) L

Heptyl Glucoside was assigned a hazard classification level of Low for single dose systemic toxicity/organ effects. The hazard score is based on no indication of specific target organ toxicity reported following oral, inhalation or dermal exposures. While some test-material related effects were observed in a few animals following dermal exposures these effects were concluded to be not of toxicological significance and were only observed to occur at very high concentrations (i.e., >2,000 mg/kg bw). Furthermore, these effects are reported for an analog compound and were not observed in tests conducted using the compound of interest. The low hazard conclusion is based on study data specific to the chemical and therefore is reported with high confidence.

Data
- Lists
  - *Authoritative: None*
  - *Screening: None*
- Measured Data

NICNAS 2015

- OECD TG 423 Acute Oral Toxicity report no signs of toxicity and no organ effects in rats dosed with 2000 mg/kg heptyl glucoside.
- OECD TG 402 Acute Dermal Toxicity reports no signs of toxicity and no organ effects in rats dosed with 2000 mg/kg heptyl glucoside.

ECHA 2023a

- In this key acute oral toxicity study following the acute toxic class method (OECD TG 423, GLP) six female fasted Sprague Dawley rats were administered a single dose of 2000 mg/kg bw of the test substance D-Glucopyranose, oligomeric, undecyl glycoside whereas another six females (control animals) received the vehicle alone (distilled water) in a stepwise procedure (three rats per step) via oral gavage (Phycher Bio Development, 2008). No mortality and no signs of systemic toxicity were observed up to the end of the 14-day observation period. Body weight gain was normal and comparable

between treated and control animals throughout the study period. Gross pathology revealed no treatment-related abnormalities in the animals. A thinning of the forestomach was noted in 2/6 animals at necropsy which was considered not to be a major sign of systemic toxicity.

- A reliable key acute dermal toxicity study performed equivalent or similar to OECD TG 402 and in compliance with GLP with the category member D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9) is available (Hill Top Biolabs, 1989). In this limit test five New Zealand White rabbits of each sex were exposed to a single dose of 2000 mg/kg bw of the test substance for 24 h via semi-occlusive dressing and observed for 14 days post-application. No severe clinical signs of toxicity were reported, and no mortalities occurred during the observation period. Partly hunched posture and slight depression occurred during the observation period. Animals showed expected gains in bodyweight over the study period and no treatment-related changes were observed at necropsy at the end of the 14-day observation period.
- A reliable supporting acute dermal toxicity study performed equivalent or similar to OECD TG 402 and in compliance with GLP with the category member D-Glucopyranose, oligomers, decyl octyl glycosides (CAS 68515-73-1) is available (Hill Top Research, 1987). In this limit test five New Zealand White rabbits of each sex were exposed to a single dose of 2000 mg/kg bw of the test substance for 24 h via semi-occlusive dressing and observed for 14 days post-application. The acute dermal LD50 value was calculated to be greater than 2000 mg/kg bw. One animal died during the 14-day observation period (Day 13). Microscopically examination revealed the Tyzzer´s disease as cause of death. Test substance-related clinical changes of emaciation (2/5), nasal discharge (3/5), fecal stains (5/5), yellow area throughout the site of application (5/5) and lacrimation (1/5) were recorded in the animals. Irritative effects on the skin in the form of moderate to marked erythema, mild to moderate edema, atonia, desquamation, and mild coriaceousness were most frequently observed within the animals. Body weight gain was recorded in 8/9 animals whereas 1/9 animals lost weight during the 14-day observation period. Gross pathology revealed a spotty area of hemorrhage in the lungs in 5/9 animals at the end of the observation period.

<u>CIR 2011</u>

- C10-16 Alkyl Glucoside Groups of 5 male and 5 female NZW rabbits were given a single dermal dose of g/kg bw C10-16 alkyl glucoside, 50% a.i. (as C10-16 APG; n:1.6). (Whether occlusion was used was not stated.) Slight depression, hunched posture, mild to marked erythema, and marked desquamation were observed. None of the animals died during the study.
- Female NMRI mice were given a single oral dose of 0.040 g (2 g/kg bw) caprylyl glucoside as a suspension in 0.2 ml of a 5% aq. solution of phosphatidylcholine. No toxic effects were observed during a 2-wk post-dose observation period. Growth and behavior were not affected.
-

- Estimated Data: None

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST-repeat) (Group II*) *L*

Heptyl Glucoside was assigned a hazard classification level of Low for repeated dose systemic toxicity/organ effects based on an oral NOAEL ≥1000 mg/kg bw/day reported for the analog C10-16-alkyl glycosides. No repeat dose inhalation data was located for the chemical of interest or other analogs and all available dermal studies were ≤ 2-week exposure durations and not included within the repeat dose classification. Some changes in organ weights were reported following exposures to ethyl glucoside however these changes occurred at very high dosing levels and are of questionable toxicological significance and have been discounted. The hazard score is based on a quality study using an analog compound; however, only oral data was available. Therefore, the hazard score is reported as low confidence.

Data

- Lists
  - *Authoritative: None*
  - *Screening: None*
- Measured Data

ECHA 2023a

- A key repeated dose toxicity study (90-day) with the category member D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9) performed equivalent to EU Method B.26 and in compliance with GLP (Henkel, 1989) is available. Groups of 10 Sprague-Dawley rats of each sex were administered the test material at doses of 250, 500 and 1000 mg/kg bw/day or vehicle alone (water) via oral gavage for 90 days on 5 consecutive days per week. In addition, groups of 5 rats of each sex were included as satellite control and high dose groups to assess the cumulative toxicity and reversibility of effects for a post-exposure period of 27 days. Animals were observed for mortalities and clinical signs (not further specified) twice daily. Body weights were recorded at arrival, on the first day of treatment and then weekly throughout the treatment period and before necropsy. Ophthalmoscopic examination was performed one day before necropsy in the control and high dose group. Hematology parameters were evaluated after six weeks and at study termination in all surviving animals. Clinical chemistry included aspartate aminotransferase, alanine aminotransferase, alkaline phosphatase, gamma-glutamyltransferase, glucose, urea, creatinine, cholesterol, total protein, bilirubin, sodium, chloride, potassium, and calcium and were evaluated after six weeks and at study termination in all surviving animals. No urinalysis and no neurobehavioral examination were performed. Gross pathology and histopathology were performed. Necropsy included the examination of all major organs, tissues, and body cavities. Histopathological examinations were performed on all the animals of the control and high dose groups. The histopathological examination of the glandular stomach (site of local effects) was also performed in animals of the intermediate dose groups and the satellite high dose group. No substance-related mortalities occurred during the study period. In summary, three animals died due to mistakes in blood sampling (2 males of the low dose group) and incidental gavage errors (1 female of the medium dose group).

The total body weight gain was slightly decreased during Weeks 1-7 of administration in males of the low dose group (250 mg/kg bw/day) and the medium dose group (500 mg/kg bw/day) in comparison to the control group due to lower initial weight of the above test groups. No substance-related effects on food consumption were observed during the study period. Water consumption was slightly increased in animals of the high dose group (1000 mg/kg bw/day), which might be compound related. No treatment-related changes were recorded at ophthalmological examination. No substance-related effects were observed for hematological and clinical chemistry parameters at study termination. Slight reduction in the absolute organ weights of gonads, brain, and thymus as well as slight increases in the relative organ weights of kidney and liver occurred in the treated groups, but these effects were not considered to be treatment-related since no corresponding changes in histopathology were observed. Gross pathology revealed ulcerations and edema restricted to forestomach in the high dose group. Histopathological examination revealed inflammatory edema of the submucosa as well as multiple ulcerations associated with acanthosis and proliferation of the mucous membrane of forestomach in animals of the medium and high dose groups. Based on the results of the study and in absence of any systemic and cumulative effects a sub-chronic systemic NOAEL of ≥1000 mg/kg bw/day was derived for D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9) in male and female rats.

CIR 2013

- Groups of 6 male Wistar ST rats were fed a diet in which sucrose was replaced with 10% or 20% ethyl glucoside for 39 days, bw gains, but not final bws, were statistically significantly decreased in the 20% group when compared to the control values. All animals survived until study termination. Total water intake was increased with increased ethyl glucoside consumption. In animals fed ethyl glucoside, kidney weights were statistically significantly increased and epididymal and abdominal fatty pad weights were statistically significantly decreased. The renal tubules of 2 and 4 control rats were “not dilated” and “slightly dilated,” respectively, and the renal tubules of all the rats in 10% group were “slightly dilated.” In the group fed 20% ethyl glucoside, the renal tubules of 3 rats were “slightly dilated,” while the other 3 had “moderately dilated” renal tubules. No microscopic damage to renal cells was observed.

- Estimated Data: None

Neurotoxicity (N-single) *M*

Heptyl Glucoside was assigned a hazard classification level of Moderate for single dose neurotoxicity based on reversible neurological effects (i.e., partly hunched posture, slight depression, and lacrimation) reported following dermal exposures to an analog compound. Based on the reported reversible nature of these effects a GHS Category 3 for single exposure is assigned to the compound. The hazard score is conservatively based on possible neurological effects however these studies do not specifically address neurological function. Therefore, the hazard score is reported with low confidence.

Data

- Lists
  - *Authoritative: None*
  - *Screening: None*
- Measured Data

NICNAS 2015

- OECD TG 423 Acute Oral Toxicity report no signs of toxicity and no organ effects in rats dosed with 2000 mg/kg heptyl glucoside.
- OECD TG 402 Acute Dermal Toxicity reports no signs of toxicity and no organ effects in rats dosed with 2000 mg/kg heptyl glucoside.

ECHA 2023a

- In this key acute oral toxicity study following the acute toxic class method (OECD TG 423, GLP) six female fasted Sprague Dawley rats were administered a single dose of 2000 mg/kg bw of the test substance D-Glucopyranose, oligomeric, undecyl glycoside whereas another six females (control animals) received the vehicle alone (distilled water) in a stepwise procedure (three rats per step) via oral gavage (Phycher Bio Development, 2008). No mortality and no signs of systemic toxicity were observed up to the end of the 14-day observation period. Body weight gain was normal and comparable between treated and control animals throughout the study period. Gross pathology revealed no treatment-related abnormalities in the animals. A thinning of the forestomach was noted in 2/6 animals at necropsy which was considered not to be a major sign of systemic toxicity.
- A reliable key acute dermal toxicity study performed equivalent or similar to OECD TG 402 and in compliance with GLP with the category member D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9) is available (Hill Top Biolabs, 1989). In this limit test five New Zealand White rabbits of each sex were exposed to a single dose of 2000 mg/kg bw of the test substance for 24 h via semi-occlusive dressing and observed for 14 days post-application. No severe clinical signs of toxicity were reported, and no mortalities occurred during the observation period. Partly hunched posture and slight depression occurred during the observation period. Animals showed expected gains in bodyweight over the study period and no treatment-related changes were observed at necropsy at the end of the 14-day observation period.
- A reliable supporting acute dermal toxicity study performed equivalent or similar to OECD TG 402 and in compliance with GLP with the category member D-Glucopyranose, oligomers, decyl octyl glycosides (CAS 68515-73-1) is available (Hill Top Research, 1987). In this limit test five New Zealand White rabbits of each sex were exposed to a single dose of 2000 mg/kg bw of the test substance for 24 h via semi-occlusive dressing and observed for 14 days post-application. Test substance-related clinical changes of emaciation (2/5), nasal discharge (3/5), fecal stains (5/5), yellow area throughout the site of application (5/5) and lacrimation (1/5) were recorded in the animals.

CIR 2011

- C10-16 Alkyl Glucoside Groups of 5 male and 5 female NZW rabbits were given a single

dermal dose of g/kg bw C10-16 alkyl glucoside, 50% a.i. (as C10-16 APG; n:1.6). (Whether occlusion was used was not stated.) Slight depression, hunched posture, mild to marked erythema, and marked desquamation were observed. None of the animals died during the study.
- Female NMRI mice were given a single oral dose of 0.040 g (2 g/kg bw) caprylyl glucoside as a suspension in 0.2 ml of a 5% aq. solution of phosphatidylcholine. No toxic effects were observed during a 2-wk post-dose observation period. Growth and behavior were not affected.

- Estimated Data: None

Neurotoxicity (N-repeated) (Group II*) DG

Heptyl Glucoside was assigned a hazard classification level of Data Gap for Neurotoxicity (N-repeated). No data was located for the compound of interest or analog compounds that addressed neurological or behavioral endpoints.

Data
- Lists
  - *Authoritative: None*
  - *Screening: None*
- Measured Data: None
- Estimated Data: None

Skin Sensitization (SnS) (Group II*) L

Heptyl Glucoside was assigned a hazard classification level of Low for skin sensitization based on the absence of a sensitization reaction report in a guideline study. The low hazard score is based on study data specific to the compound of interest and is supported by negative skin sensitization results reported for analog substances. This hazard conclusion is therefore reported with high confidence.

Data
- Lists
  - *Authoritative: None*
  - *Screening: None*
- Measured Data: None
- Estimated Data: None

NICNAS 2015

- OECD TG 406 Skin Sensitization – Magnusson & Kligman Test Method The results showed that the test substance did not cause skin sensitization in guinea pigs under the testing condition There was no evidence of reactions indicative of skin sensitization to

the notified chemical under the conditions of the test.

ECHA 2023a

- The skin sensitization potential of the whole range of alcohol polyglycosides was evaluated in the guinea pig maximization test according to the Magnusson Kligman and in the non-adjuvant Buehler test protocol in guinea pigs. In summary, all of the six studies conducted with hexyl-D-glucoside, C8-10-alkyl glycosides and C10-16-alkyl glycosides showed that the APGs have no skin sensitizing potential.

ECHA 2023b

- The skin sensitizing properties of D-Glucopyranose, oligomeric, undecyl glycoside were tested in a non-GLP study performed equivalent or similar to OECD TG 406 using the Guinea pig maximization test (GPMT, EVIC-CEBA, 1993). The GPMT test was performed on 30 female Dunkin-Hartley guinea pigs. For the intradermal and epicutaneous inductions, the test item concentration was 0.5% active ingredient (v/v in distilled water) whereas 0.25% and 0.5% (a.i.) (v/v in distilled water) formulations were selected for the challenge exposure. At the beginning of the induction exposure 20 test animals and 10 control animals were intradermally treated with 0.5% (a.i.) of the test substance and vehicle (Day 0), respectively, followed by a topical induction (0.5% a.i.) under occlusive conditions one week later. On Day 20 all animals were challenged for 24 h with the test substance at a concentration of 0.25% and 0.5% (a.i.). under occlusive conditions. Skin reactions of all animals were evaluated 48 and 72 hours after challenge administration. No mortalities occurred and no signs of systemic toxicity were observed during the study period. Neither erythema nor edema formation was recorded at any concentration in any animal. The mean weight gain calculated for the treated animals during the test period was not significantly different from that of the control animals. No information on periodically reliability checks of positive control animals is available. Thus, under the conditions of the test, the test substance revealed no skin sensitizing properties.
- In another study, the skin sensitizing properties of the category member D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9) were tested in a study performed equivalent or similar to OECD TG 406 and in compliance with GLP using the Guinea pig maximization test (GPMT, Henkel, 1988). The GPMT test was performed on 40 female Pirbright-Hartley guinea pigs. For the intradermal and epicutaneous inductions, the initial test item concentration was 0.1% (a.i.) (v/v in 20% 1,2-propylene glycol) and 10% (a.i.) (v/v in 100% 1,2-propylene glycol) whereas a 1.25% and 2.5% (a.i.) (v/v in 100% 1,2-propylene glycol) formulation was selected for the epicutaneous induction and the challenge exposure. At the beginning of the induction exposure 20 test animals and 20 control animals were either intradermally treated with 0.1% (a.i.) of the test substance or vehicle (Day 0), followed by a topical induction of 10% (a.i.) of the test substance under occlusive conditions one week later. On Day 22 all animals were challenged with the test substance at a concentration of 1.25% and 2.5% (a.i.). Skin reactions of all animals were evaluated 48 and 72 hours after challenge administration. No mortalities occurred and no signs of systemic toxicity were observed during the study period. Slight erythema formation was recorded in 1/20 control animals 48 h after challenge administration (1.25% (a.i.)) which was still present after 72 hours. No erythema were recorded at animals of the test group following an

induction exposure of 0.1% (a.i.) and challenge exposure of 1.25% (a.i.), neither 48 nor 72 hours after challenge exposure. Slight erythema formation was recorded in 3/20 control animals 48 h after challenge administration (2.5% (a.i.)) which was still present in 1/20 animals after 72 hours. Following an induction exposure of 0.1% (a.i.) of the test substance only 1/20 test group animals showed slight erythema formation 24 and 48 after challenge exposure (2.5% (a.i.)). No edema formation was recorded at any animal. No information on periodically reliability checks of positive control animals is available. Thus, under the conditions of the test, the test substance revealed no skin sensitizing properties.

- In another study, the skin sensitizing properties of the category member D-Glucopyranose, oligomers, branched and linear C9-11-alkyl glycosides (CAS 157707-87-4) were tested in a non-GLP study performed equivalent or similar to OECD TG 406 using the Guinea pig maximization test (GPMT, Drug Safety Testing Center, 1988). The GPMT test was performed on 30 female Hartley guinea pigs. For the intradermal and epicutaneous inductions, the initial concentration was 0.3% (a.i.) (v/v in physiological saline) whereas 0.5%, 1% and 3% (a.i.) (v/v in physiological saline) formulations were selected for the epicutaneous induction and the challenge exposure. At the beginning of the induction exposure 20 test animals and 10 control animals were either intradermally treated with 0.5% (a.i.) test substance or vehicle (Day 0), followed by a topical induction of 0.5% (a.i.) of the test substance under occlusive conditions one week later. On Day 22 all animals were challenged with the test substance at concentrations of 0.5%, 1% and 3% (a.i.). Skin reactions of all animals were evaluated 48 and 72 hours after challenge administration. No mortalities occurred and no signs of systemic toxicity were observed during the study period. Neither erythema nor edema formation was recorded at any concentration in any animal. No information on periodically reliability checks of positive control animals is available and no pilot study for selection of appropriate concentrations for induction and challenge exposure was performed. In summary, under the conditions of the test, the test substance revealed no skin sensitizing properties. Thus, under the conditions of the test, the test substance revealed no skin sensitizing properties.

Respiratory Sensitization (SnR) (Group II*)

Heptyl Glucoside was assigned a hazard classification level of Data Gap for respiratory sensitization based on lack of adequate studies. No data was located for the compound of interest or analog compounds that addressed respiratory sensitization (SnR).

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Data

- Lists
  - *Authoritative: None*
  - *Screening: None*
- Measured Data: None
- Estimated Data: None

Skin Irritation/Corrosivity (IrS) *H*

Heptyl Glucoside was assigned a hazard classification level of High for skin irritation/corrosivity based on weight of evidence using an in vitro study for the

compound of interest and studies for analog compounds that indicate slight reversible erythema formation following dermal exposures. One study reported a score of 2.9 for erythema more severe effects, however, the effects were reported as fully reversible within 17 days and therefore a GHS category 2 for skin irritation has been assigned. The hazard conclusion is based on reliable data, however, there is evidence that irritation potential is influenced by the alkyl chain length. Without in vivo study data specific to the compound of interest the hazard score is assigned with low confidence.

Data

- Lists
    - *Authoritative: None*
    - *Screening: None*
- Measured Data

NICNAS 2015

- OECD TG 439 In vitro Skin Irritation: Reconstructed Human Epidermis Test Method The notified chemical (Heptyl glucoside) was non-irritating to the skin under the conditions of the test.

ECHA 2023a

- A non-GLP skin irritation study with D-Glucopyranose, oligomeric, undecyl glycoside is available and was performed equivalent or similar to OECD TG 404 (BIOGIR, 1992a). In the study three rabbits of unknown strain were exposed to 0.5 mL of the test material (10% a.i.). Skin reactions were evaluated 24 and 72 hours post-application. No scoring was performed after 48 hours; therefore, the same irritation scores as after 24 hours were assumed. Slight erythema formation (grade 1) was recorded in all animals 24 h after start of exposure. These effects were fully reversible in all animals within 72 hours (mean value over 24, 48 and 72 h: 0.67). No edema formation was detected in any animal. Based on the results of the study the test item should be considered as non-irritating when applied as 10% (a.i.) formulation.
- A non-GLP skin irritation study with the category member D-Glucopyranose, oligomeric, C10-16-alkyl glycosides is available and was performed according to OECD TG 404 and in compliance with GLP (Henkel, 1988). In the study four Kleinrusse rabbits were exposed to 0.5 g of the test material (60% a.i.) for 4 hours under occlusive conditions. Skin reactions were evaluated 1, 24, 48 and 72 hours and 7, 10, 17 and 21 days post-application. Slight to moderate skin erythema (grade 1-3) and edema (grade 1-3) as well as eschar formation were observed in all animals after treatment. These reactions were fully reversible within 17 days. The mean values over 24, 48 and 72 hours were calculated to be 2.9 for erythema and 2.1 for edema. No further local or systemic effects were observed. Based on the results of the study the test item should be considered as irritating when applied as 60% (a.i.) formulation.
- Another non-GLP study investigating the skin irritating potential of the category member D-Glucopyranose, oligomers, branched and linear C9-11-alkyl glycosides performed equivalent or similar to OECD TG 404 is available (Drug Safety Testing Center, 1988). Groups of six Japanese White rabbits per dose were exposed to the test substance undiluted (50% a.i.) or at concentrations of 30% (w/v) (15% a.i.) and 3% (w/v) (1.5% a.i.)

in phosphate buffered saline (1/15 M pH 7.2), respectively for 24 h under occlusive conditions. Skin reactions were examined, and the changes were graded according to the Draize scoring system 3, 24 and 48 hours post-application. The mean erythema score over 24, 48 and (predicted) 72 h and all animals was 0.7 for the undiluted test substance, and effects were not fully reversible within 48 h. However, this observation period was insufficient to assess the full reversibility of skin irritation. No erythema was noted after exposure to the test substance at 3 and 30% and no edema was seen at any concentration tested. The test item is considered as not irritating when applied as 50% (a.i.) formulation.

CIR 2011

- APGs of varying chain length (C8/10 to C12/16; 15-70% a.i.) demonstrated a structure-response relationship, with irritation potential decreasing with increasing chain length, and, independent of the degree of polymerization, the irritation was mostly concentration-dependent. The primary dermal irritation indices (PDIIs) ranged from 0.0 to 4.6 in rabbits. (A PDII of 2 was considered a positive responder).
- In clinical studies, the dermal irritation of decyl, lauryl, and coco-glucosides was evaluated in epicutaneous patch (2.0% a.i.) and soap chamber tests (1.0% a.i.), and decyl glucoside was evaluated in an SIOPT (0.5% a.i.). At most, these ingredients were slightly irritating.

- Estimated Data: None

Eye Irritation/Corrosivity (IrE): *vH*

Heptyl Glucoside was assigned a hazard classification level of Very High for eye irritation/corrosivity based on a study using the chemical of interest which reported moderate corneal opacity and corneal neovascularization that persisted throughout the 21-day observation period. In alternative system studies for ocular irritation, the irritation potential of the compound of interest and analog compounds were non to slightly irritating. In addition, studies in analog substances suggest a threshold exists for ocular irritation potential and that ocular irritation is influenced by alkyl chain length. While the hazard conclusion is based on study data using the compound of interest, mixed results are reported using alternative systems and analogs and the irritation potential appears to be concentration dependent. Therefore, the hazard score is reported with low confidence.

Data
- Lists
    - *Authoritative: None*
    - *Screening: None*
- Measured Data

NICNAS 2015

- In an OECD TG 405 Acute Eye Irritation/Corrosion a moderate redness of the conjunctivae was observed at 24 h and was reversible on day 7. A congestion or hemorrhage of the iris was observed at 1 h or 24 h and was reversible between days 7 and 14. A moderate corneal opacity was observed in two animals at 24 h and in one animal on the last day of the test. A corneal neovascularization was observed on day 14 and day 21 in one animal. The notified chemical caused irreversible effects to the eye.
- OECD TG 437 Bovine Corneal Opacity and Permeability Test Method for Identifying Ocular Corrosives and Severe Irritants The test substance was provided at a 10% solid concentration and was diluted in the vehicle at 10% concentration at the request of the notifier for an overall concentration of 1% of the test substance. The positive control gave an in vitro irritation score that was reportedly within two standard deviations of the current historical mean confirming the validity of the test system. The study authors concluded that the test substance does not require classification for eye irritation.

ECHA 2023a

- A non-GLP eye irritation study performed equivalent or similar to OECD TG 405 with D-Glucopyranose, oligomeric, undecyl glycoside is available. For the assessment of the eye irritation properties 0.1 mL of the test substance (10% a.i.) was instilled in the eyes of three rabbits of unknown strain (right eye was washed after 30 sec, left eye remained unwashed). The eyes were examined, and the changes were graded according to the Draize scoring system 1, 24, 48 and 72 hours and 4 and 7 days post-application. Only individual scores for conjunctivae, iris, corneal opacity and chemosis effects of the left eye (without rinsing) were evaluated. Corneal opacity was noted in 2/3 animals (grade 11) 1 h after application of the test material.24 h after application of the test material corneal opacity was observed in 3/3 animals (grade 2). These effects were fully reversible within 4 days (1/3 animals) and 7 days (2/3 animals), respectively. Iris effects (grade 1) were recorded in 1/3 animals 24 h after application of the test material but being fully reversible within 48 h. Conjunctivae effects (grade 1) were observed in 3/3 animals 1 h, 24, 48 and 72 h after application of the test material. These effects were fully reversible within 4 days (2/3 animals) and 7 days (1/3 animals), respectively. Chemosis was observed in 1/3 (grade 1) and 2/3 (grade 2) animals 1 h after application of the test material, but these effects were fully reversible within 72 h (2/3 animals with initially grade 2) and 4 days (1/3 animals with initially grade 1). Any effects observed had fully reversed at the end of the observation period. Based on the study results and according to EU classification criteria, the test substance is considered to be irritating to the eye when applied as 10% (a.i.) formulation, whereas classification as Eye Dam. 1 is assumed at higher concentrations (>10% a.i.).

ECHA 2023b

- The eye irritation toxicity of the compounds in this category is predicted to require the labelling "risk of serious damage to eyes" (R41), since all tested alkyl polyglycosides, e.g., C8-10-alkyl glycosides and C10-16-alkyl glycosides, display a severe eye irritating potential.

CIR 2013

- In alternative system studies for ocular irritation, the irritation potential of 0.6% to 3.0% ai decyl, lauryl, and coco-glucosides, and of C10-16 alkyl glucosides (pH 7, 11.5; concentration not stated), were non to slightly irritating. Caprylyl/capryl glucoside (concentration not stated) was highly irritating in a hen's egg test-chorioallantoic membrane (HET-CAM) assay. In a HET-CAM study with APGs of varying proportions of alkyl chain length, the ocular irritation potential increased with the increased proportion of shorter chain APGs. In studies using rabbits, neutralized lauryl glucoside produced slight ocular reactions. Caprylyl/capryl glucoside was severely irritating to rabbit eyes when tested undiluted; the irritation threshold value was 10% for 30% ai caprylyl/capryl glucoside and 5% for 60% ai caprylyl/capryl glucoside.

- Estimated Data: None

ECOTOXICITY (ECOTOX)

Acute Aquatic Toxicity (AA): L

Heptyl Glucoside was assigned a hazard classification level of Low for acute aquatic toxicity based on studies reporting LC50 >100 for both aquatic invertebrates and algal growth. This conclusion is supported by results using the analogs hexyl D-glucoside and undecyl glucoside which indicate LC50 and EC50 values >100 mg/L for all three trophic levels (i.e., fish, invertebrates, and algae). The hazard conclusion is based on study data and is therefore reported with high confidence.

Data
- Lists
    - *Authoritative: None*
    - *Screening: None*
- Measured Data

NICNAS 2015

- EC50 >100 mg/L is reported for daphnia- D-Glucopyranose, oligomeric, heptyl glycosides (INCI Name: Heptyl glucoside)
- EC50 = 107.8 mg/L reported for algal toxicity D-Glucopyranose, oligomeric, heptyl glycosides (INCI Name: Heptyl glucoside)

ECHA 2023a

- A study was performed to assess the effect of the test material on the growth of the green alga Scenedesmus subspicatus. The method followed that described in the OECD Guidelines for Testing of Chemicals (1984) No 201, "Alga, Growth Inhibition Test". Scenedesmus subspicatus was exposed to an aqueous dispersion of the test material at concentrations of 62.5, 125, 250, 500 and 1000 mg active ingredient per liter (mg a.i./L), with three replicate flasks per concentration, for 72 hours under constant illumination and shaking at a temperature of 24 +/- 1 °C. Samples of the algal

populations were removed daily and cell concentrations determined for each control and treatment group. Exposure of Scenedesmus subspicatus to the test material gave a nominal EC50 (72 h) value of 180 mg a.i./L and an EC50 (0 - 72 h) value of 780 mg a.i./L. The No Observed Effect Concentration was found to be nominally 125 mg a.i./L. .

- In this study the acute toxicity to first instar Daphnia magna was studied as a static test. The study was performed according to OECD guideline 202 and under GLP. After 24 hours exposure no immobilization was observed in any test concentration. Only after 48 hours a dose-response immobilization was observed for concentrations >= 320 mg a.i. /L. The EC50 (48 hours) was therefore determined at nominally 490 mg a.i. /L, while the NOEC (48h) was determined at 180 mg a.i. /L.
- In this study the acute toxicity of the test substance to first instar Daphnia magna was studied as a static test. The study was performed according to OECD guideline 202 and under GLP and was a limit test. Based on nominal concentration only, the NOEC (48 h) was concluded >= 100 mg/L, and the EC50 (48h) was > 100 mg/L.
- In this study the acute toxicity to rainbow trout was studied as a semi static test. The study was performed according to OECD guideline 203 and under GLP. Apart from mortality, sub-lethal effects (swimming at bottom or surface, loss of equilibrium, moribund animals) were noted in concentrations >= 320 mg a.i./L. Based on nominal concentrations only, the NOEC (96h) was concluded 180 mg a.i./L, and the LC50 (96h) was 420 mg a.i./L.
- In this study the acute toxicity to rainbow trout was studied as a semi static test. The study was performed according to OECD guideline 203 and under GLP and was a limit test. Based on nominal concentration only, the NOEC (96 h) was concluded >= 100 mg/L, and the LC50 (96 h) was > 100 mg/L

ECHA 2023b

- In an OECD Guideline 203 (Fish, Acute Toxicity Test) as adapted by OSPAR commission (ref number 2005-11) protocol for a fish acute toxicity test amended March 2005 using turbot (flatfish) an LL50 > 37.6 mg/L is reported.
- In an OECD Guideline 203 (Fish, Acute Toxicity Test) using zebra fish an LC50 > 100 mg/L is reported.
- In an ISO 14669 (1999) Water Quality - Determination of acute lethal toxicity to marine copepods (Copepoda; Crustacea) using copepod an LL50 > 60.19 mg/L is reported for D-Glucopyranose, oligomers, undecyl glycosides.
- In an OECD Guideline 202 (Daphnia sp. Acute Immobilisation Test) using Daphnia magna an LC50 > 100 mg/L is reported for D-Glucopyranose, oligomers, undecyl glycosides.
- In an OECD Guideline 201 (Alga, Growth Inhibition Test) using Pseudokirchneriella subcapitata an LC50 > 100 mg/L is reported for D-Glucopyranose, oligomers, undecyl glycosides.
- Short-term toxicity to fish is well studied for the category of alkyl polyglycosides and includes studies with substances ranging from D-Glucopyranose, oligomeric, butyl glycoside to D-Glucose, reaction products with alcohols C16-18 (even numbered) (excess), covering a variety of both freshwater and marine species. Alkyl polyglycosides of chain lengths from C4 to C8-10 seem to have low to moderate toxicity, whereas substances from C9-11 to C10-16 are more toxic. Toxicity of D-Glucose, reaction products with alcohols C16-18 (even numbered) (excess) could not be observed, which

can be explained by reduced bioavailability as a consequence of the low water solubility. The 96-hour LC50 values for fish determined for alkyl polyglycosides vary from 2.95 mg/L for D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9) up to 420 mg/L for D-Glucopyranose, oligomers, hexyl glycosides.

- Estimated Data: None

Chronic Aquatic Toxicity (CA): M

Heptyl Glucoside was assigned a hazard classification level of Moderate for chronic aquatic toxicity based on measured data in analogs indicating NOEC and EC10 values between 1 < 10 mg/L in all three trophic levels. The conclusion is based on study data using quality analogs and is therefore reported with high confidence.

Data

- Lists
  - *Authoritative: None*
  - *Screening: None*
- Measured Data

ECHA 2023a

- The 72-h NOEC values for algae range from 2 mg/L for D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9) to 125 mg/L for D-Glucopyranose, oligomers, hexyl glycosides, based on key studies.
- One long-term test on aquatic invertebrates is available for the member substance D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9), with a resulting EC10 value of 1.76 mg/L. As D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9) represents the worst case regarding acute aquatic toxicity, this study is applied as source for read-across for the other members of the alkyl polyglycosides category. Specifically, in a 21 d test with Daphnia magna according to the OECD guideline 202 part II (Stelter, 1995). The test design was semi-static with a daily renewal of the test substance und growth medium. Concentrations up to 16 mg/L were used for the test. The test exhibited an EC10 value (21 d) of 1.76 mg a.i./L for the endpoint mortality and a NOEC (21 d) of 2 mg a.i./L for the endpoint reproduction, respectively.
- One long-term test on fish is available for D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9), with a resulted NOEC value of 1.8 mg/L. As D-Glucopyranose, oligomeric, C10-16-alkyl glycosides (CAS 110615-47-9) represents the worst case regarding acute aquatic toxicity, this study is applied as source for read-across for the other members of the alkyl polyglycosides category. Specifically, the toxicity of the substance to the zebrafish Brachydanio rerio was tested in a prolonged fish toxicity test according to the OECD guideline 204 ("Fish, prolonged toxicity test: 14-day study") for 28 days. This test can be used as a long-term test because the following criteria are fulfilled: the duration is 28 days; the tested fish life stage is equal to OECD 215 and additional parameters like behavior and growth were investigated (according to “Guidance Document on Aquatic Ecotoxicology” published by the European Commission (2002)). The test exhibited a NOEC of 1.8 mg a.i./L after 28 days for the

endpoint mortality and a NOEC of 3.2 mg a.i./L for the endpoint growth, respectively. No behavioral abnormalities were observed in the non-toxic concentrations of the test substance.

- Estimated Data: None

ENVIRONMENTAL FATE (FATE)

Persistence (P): vL

Heptyl Glucoside was assigned a hazard classification level of very low for persistence based on analytical testing using the compound of concern. This hazard conclusion is supported by results measured with analogs hexyl-D-glucoside and undecyl glucoside which showed both substances meet the 10-day window in “Ready Biodegradation”. The hazard conclusion is based on study data using high quality analogs and modeled estimates and is therefore reported with high confidence.

Data

- Lists
  - *Authoritative: None*
  - *Screening: None*
- Measured Data

NICNAS 2015

- Heptyl glucoside- OECD TG 301 F Ready Biodegradability: Manometric Respirometry Test. The percentage degradation of the reference compound, sodium benzoate, surpassed the threshold level of 60% by 7 days (> 65%) and neared 80% degradation by 14 days. Therefore, the test indicates the suitability of the inoculums. The notified chemical attained 82.25% degradation by 28 days and attained the threshold level of 60% within the 10-day window. Therefore, the notified chemical can be classified as readily biodegradable according to the OECD (301F) guideline.

ECHA 2023a

- Ready biodegradability was determined for hexyl-D-glucoside using the Closed Bottle test performed according to slightly modified OECD, EU and IS0 Test Guidelines, and in compliance with the OECD principles of Good Laboratory Practice. The test substance was biodegraded 71% at day 28 in the Closed Bottle test. Over 60% biodegradation was achieved within a period of 10 days immediately following the attainment of 10% biodegradation. Hence the test substance should be classified as readily biodegradable. The test is valid as shown by an endogenous respiration of 1.1 mg/L and by the total mineralization of the reference compound, sodium acetate. Sodium acetate was degraded 70% of its theoretical oxygen demand after 14 days. Finally, the most important criterion was met by oxygen concentrations >0.5 mg/L in all bottles during the test period. is deemed to be not persistent in the environment as it is readily biodegradable and moreover hydrolysis is not a relevant pathway according to an

OECD 111 screening test. Therefore, the substance is not expected to be persistent in the environment. Evaporation from the water phase to the air can be precluded due to the low Henry's law constant (5.98E-017 Pa m3/mol – 6.51E-009 Pa m3/mol). Therefore, water is expected to be the main compartment of substance distribution. However, if emitted into the air the substance is susceptible to indirect photodegradation (DT50 < 24 h).

- In order to assess the biotic degradation of hexyl-D-glucoside, a ready biodegradability test was performed which allows the biodegradability to be measured in an aerobic aqueous medium. The ready biodegradability was determined in the Closed Bottle test performed according to slightly modified OECD, EEC and IS0 Test Guidelines, and in compliance with the OECD principles of Good Laboratory Practice. The test substance caused no reduction in the endogenous respiration. The test substance is therefore considered to be non-inhibitory to the inoculum. The test substance was biodegraded 71% at Day 28 in the Closed Bottle test. Hence this compound should be classified as readily biodegradable. The test is valid as shown by an endogenous respiration of 0.7 mg/L and by the total mineralization of the reference compound, sodium acetate. Sodium acetate was degraded 85% of its theoretical oxygen demand after 14 days. Finally, the most important criterion was met by oxygen concentrations >0.5 mg/L in all bottles during the test period.
- In a study by IBACON GmbH (2008) the ready biodegradability of undecyl glucoside according to the OECD guideline 301 F (and GLP) was investigated. This study was chosen as the key study. A non-adapted, activated sludge from a domestic sewage treatment plant was used as inoculum and was exposed to an initial nominal test substance concentration of 102 mg/L (96 mg/L based on ThOD(NH4)). After 28 d test duration, 85% degradation of the test substance (ThOD(NH4) based on O2 consumption) was observed. The 10-day window criterion was fulfilled. A toxicity control containing both, reference substance (sodium benzoate, 170 mg/L based on ThOD(NH4)) and test substance did not indicate inhibitory effects to the inoculum, as 78% biodegradation, based on ThOD(NH4), of the reference item took place within 14 d.
- Estimated Data: None

Bioaccumulation (B): vL

Heptyl Glucoside was assigned a hazard classification level of very Low for bioaccumulation based on a report logKow of ≤ 3. This is a measured value reported for a high quality analog and therefore is reported as high confidence.

Data

- Lists
  - *Authoritative: None*
  - *Screening: None*
- Measured Data

ECHA 2023b

- No experimental studies involving the bioaccumulation potential of undecyl glucoside are available however, according to column 2 of Annex IX REACH regulation 1907/2006, studies on the accumulation in aquatic species do not need to be conducted

as the substance has a log Kow of less than or equal to three, and therefore a low potential for bioaccumulation is expected.

- Estimated Data:

ECHA 2023b

- The BCF (bioconcentration factor) values calculated for the main constituents of the substance with the reliable QSAR model (BCFBAF v3.01, EPI Suite). BCF values of 0.8931 to 10.18 L/Kg were estimated using the Arnot-Gobas method, including biotransformation (BCFBAF v3.01, EPI suite). The BCF values are well below 2000, indicating a low potential for bioaccumulation. Furthermore, the substance can be digested by common metabolic pathways, which enhances the assumption of no bioaccumulation in organisms.

-

PHYSICAL HAZARDS (PHYSICAL)

Reactivity (Rx): *L*

Heptyl Glucoside was assigned a hazard classification level of Low for reactivity based on the absence of chemical groups that are associated with explosivity or oxidizing properties. The hazard score is based on the chemical structure and professional judgement and therefore is reported as low confidence.

Data
- Lists
  - *Authoritative: None*
  - *Screening: None*
- Measured Data

ECHA 2023a

- Hexyl D-glucoside is categorized as non-explosive as there are no chemical groups associated with explosive properties present in the molecule of D-glucopyranose, oligomers, and hexyl glucosides. Undecyl glucoside was also classified as non-explosive because no chemical groups associated with explosive properties are present in the molecule. The available data on explosive properties of the test substance did not meet the criteria for classification according to Regulation (EC) No. 1272/2008, which is conclusive but not sufficient for classification. Both suitable analogs are incapable of reacting exothermically with combustible materials, and are classified as non-oxidizing, per the same criteria for classification as flammability.

- Estimated Data: None

Flammability (F): L

Heptyl Glucoside was assigned a hazard classification level of Low for flammability based on flammability tests conducted using the analog hexyl D-glucoside and undecyl glucoside. This hazard conclusion is based on available study data for high quality analogs and is therefore reported with high confidence.

Data

- Lists
    - *Authoritative: None*
    - *Screening: None*
- Measured Data

ECHA 2023a

- Hexyl-D-glucoside did not ignite and propagate combustion either by burning with flame or smoldering, indicating that it is not considered as highly flammable. In the screening test the gas flame was applied for 2 minutes to one end of the substance train, but no ignition and no propagation of combustion occurred. Only melting took place at the part of the substance that was exposed to the flame. The flammability of the test substance was determined according to EC regulation No. 440/2008, Guideline A.10.

ECHA 2023b

- Undecyl glucoside was classified as non-flammable, having no pyrophoricity, and no flammability on contact with water. The justification of these classifications is based on the chemical structure and experience in handling and use. During the preliminary test, the test item melted. Neither propagation nor ignition was observed. The test was performed using the United Nations Recommendations on the Transport of Dangerous Goods Manual of tests and Criteria Fifth revised edition (2009) Test N.1 (Part III, Section 33.2.1.4). Both analogs test results and classifications were performed, reported, and gathered from the ECHA.

- Estimated Data: None

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APPENDIX A: HAZARD CLASSIFICATION ACRONYMS

(Alphabetical order)

(AA) Acute Aquatic Toxicity

(AT) Acute Mammalian Toxicity

(B) Bioaccumulation

(C) Carcinogenicity

(CA) Chronic Aquatic Toxicity

(D) Developmental Toxicity

(E) Endocrine Activity

(F) Flammability

(IrE) Eye Irritation/Corrosivity

(IrS) Skin Irritation/Corrosivity

(M) Mutagenicity and Genotoxicity

(N) Neurotoxicity

(P) Persistence

(R) Reproductive Toxicity

(Rx) Reactivity

(SnS) Sensitization- Skin

(SnR) Sensitization- Respiratory

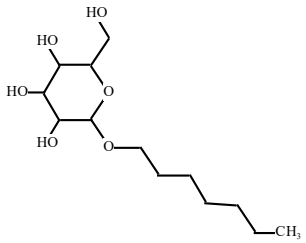
(ST) Systemic/Organ Toxicity

APPENDIX B – MODELING RESULTS

Attach:

- **EPISuite Results for Heptyl Glucoside (CAS# 100231-64-9)**

EPI Suite Results for CAS 100231-64-9




```
SMILES : O1C(OCCCCCCC)C(O)C(O)C(O)C1CO
CHEM   :
MOL FOR: C13 H26 O6
MOL WT : 278.35
------------------------------ EPI SUMMARY (v4.11) --------------------------
Physical Property Inputs:
Log Kow (octanol-water):   ------
Boiling Point (deg C)  :   ------
Melting Point (deg C)  :   ------
Vapor Pressure (mm Hg) :   ------
Water Solubility (mg/L):   ------
Henry LC (atm-m3/mole) :   ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) =  0.44
Log Kow (Exper. database match) =  0.73
Exper. Ref:  SANGSTER (1993)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C):  434.26  (Adapted Stein & Brown method)
Melting Pt (deg C):  166.33  (Mean or Weighted MP)
VP(mm Hg,25 deg C):  9.3E-011  (Modified Grain method)
VP (Pa, 25 deg C) :  1.24E-008  (Modified Grain method)
Subcooled liquid VP: 2.66E-009 mm Hg (25 deg C, Mod-Grain method)
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: 3.54E-007 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L):  3898
log Kow used: 0.73 (expkow database)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) =  1e+006 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method :   8.53E-014  atm-m3/mole  (8.65E-009 Pa-m3/mole)
Group Method:   1.69E-023  atm-m3/mole  (1.71E-018 Pa-m3/mole)
For Henry LC Comparison Purposes:
User-Entered Henry LC:  not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC:  8.738E-015 atm-m3/mole  (8.854E-010 Pa-m3/mole)
VP:   9.3E-011 mm Hg (source: MPBPVP)
WS:   3.9E+003 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used:  0.73  (exp database)
Log Kaw used:  -11.458  (HenryWin est)
Log Koa (KOAWIN v1.10 estimate):  12.188
Log Koa (experimental database):  None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model)         :   0.6637
Biowin2 (Non-Linear Model)     :   0.1843
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model):   3.5049  (days-weeks  )
Biowin4 (Primary Survey Model) :   4.2135  (days        )
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model)    :   0.9401
Biowin6 (MITI Non-Linear Model):   0.6617
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model):  0.8345
Ready Biodegradability Prediction:   YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled):  3.55E-007 Pa (2.66E-009 mm Hg)
Log Koa (Koawin est  ): 12.188
Kp (particle/gas partition coef. (m3/ug)):
Mackay model           :  8.46
Octanol/air (Koa) model:  0.378
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model     :  0.997
Mackay model           :  0.999
Octanol/air (Koa) model:  0.968
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Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant =  78.6197 E-12 cm3/molecule-sec
Half-Life =     0.136 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life =     1.633 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
0.998 (Junge-Pankow, Mackay avg)
0.968 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc    :  10  L/kg (MCI method)
Log Koc:  1.000       (MCI method)
Koc    :  2.113  L/kg (Kow method)
Log Koc:  0.325       (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
Log Biotransformation Half-life (HL) = -1.8076 days (HL = 0.01557 days)
Log BCF Arnot-Gobas method (upper trophic) = 0.044 (BCF = 1.106)
Log BAF Arnot-Gobas method (upper trophic) = 0.044 (BAF = 1.106)
log Kow used: 0.73 (expkow database)

Volatilization from Water:
Henry LC:  8.53E-014 atm-m3/mole  (estimated by Bond SAR Method)
Half-Life from Model River: 1.145E+010  hours   (4.771E+008 days)
Half-Life from Model Lake : 1.249E+011  hours   (5.205E+009 days)

Removal In Wastewater Treatment:
Total removal:               1.87  percent
Total biodegradation:        0.09  percent
Total sludge adsorption:     1.78  percent
Total to Air:                0.00  percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model:
Mass Amount    Half-Life    Emissions
(percent)        (hr)       (kg/hr)
Air       0.00109         3.26         1000
Water     28.1            208          1000
Soil      71.8            416          1000
Sediment  0.0592          1.87e+003    0
Persistence Time: 414 hr
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- **ECOSAR Results for Chemical Name (CASRN)**
- **Other**