SCREENING-LEVEL HAZARD CHARACTERIZATION OF HIGH PRODUCTION VOLUME CHEMICALS

CHEMICAL CATEGORY NAME:
C_7 to C_9 Aliphatic Aldehydes and Carboxylic Acids

SPONSORED CHEMICALS

Heptanal	**CAS No. 111-71-7**
Heptanoic Acid	**CAS No. 111-14-8**
Octanal	**CAS No. 124-13-0**
Nonanal	**CAS No. 124-19-6**

SUPPORTING CHEMICALS

2,6-Dimethyl-5-heptenal	**CAS No. 106-72-9**
Decanal	**CAS No. 112-31-2**
Nonanoic acid	**CAS No. 112-05-0**
Octanoic acid	**CAS No. 124-07-2**
Hexanal	**CAS No. 66-25-1**

August 2007

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SCREENING-LEVEL HAZARD CHARACTERIZATION OF HIGH PRODUCTION VOLUME CHEMICALS

The High Production Volume (HPV) Challenge Program[1] is a voluntary initiative aimed at developing and making publicly available screening-level health and environmental effects information on chemicals manufactured in or imported into the United States in quantities greater than one million pounds per year. In the Challenge Program, producers and importers of HPV chemicals voluntarily sponsor chemicals; sponsorship entails the identification and initial assessment of the adequacy of existing toxicity data/information, conducting new testing if adequate data do not exist, and making both new and existing data and information available to the public. Each complete data submission contains data on 18 internationally agreed to "SIDS" (Screening Information Data Set[1,2]) endpoints that are screening-level indicators of potential hazards (toxicity) for humans or the environment.

The Environmental Protection Agency's Office of Pollution Prevention and Toxics (OPPT) is evaluating the data submitted in the HPV Challenge Program on approximately 1400 sponsored chemicals. OPPT is using a hazard-based screening process to prioritize review of the submissions. The hazard-based screening process consists of two tiers described below briefly and in more detail on the Hazard Characterization website[3].

Tier 1 is a computerized sorting process whereby key elements of a submitted data set are compared to established criteria to "bin" chemicals/categories for OPPT review. This is an automated process performed on the data as submitted by the sponsor. It does not include evaluation of the quality or completeness of the data.

In Tier 2, a screening-level hazard characterization is developed by EPA that consists of an objective evaluation of the quality and completeness of the data set provided in the Challenge Program submissions. The evaluation is performed according to established EPA guidance[2,4] and is based primarily on hazard data provided by sponsors. EPA may also include additional or updated hazard information of which EPA, sponsors or other parties have become aware. The hazard characterization may also identify data gaps that will become the basis for a subsequent data needs assessment where deemed necessary. Under the HPV Challenge Program, chemicals that have similar chemical structures, properties and biological activities may be grouped together and their data shared across the resulting category. This approach often significantly reduces the need for conducting tests for all endpoints for all category members. As part of Tier 2, evaluation of chemical category rationale and composition and data extrapolation(s) among category members is performed in accord with established EPA[2] and OECD[5] guidance.

The screening-level hazard characterizations that emerge from Tier 2 are important contributors to OPPT's existing chemicals review process. These hazard characterizations are technical documents intended to support subsequent decisions and actions by OPPT. Accordingly, the documents are not written with the goal of informing the general public. However, they do provide a vehicle for public access to a concise assessment of the raw technical data on HPV chemicals and provide information previously not readily available to the public. The public, including sponsors, may offer comments on the hazard characterization documents.

The screening-level hazard characterizations, as the name indicates, do not evaluate the potential risks of a chemical or a chemical category, but will serve as a starting point for such reviews. In 2007, EPA received data on uses of and exposures to high-volume TSCA existing chemicals, submitted in accordance with the requirements of the Inventory Update Reporting (IUR) rule. For the chemicals in the HPV Challenge Program, EPA will review the IUR data to evaluate exposure potential. The resulting exposure information will then be combined with the screening-level hazard characterizations to develop screening-level risk characterizations[4,6]. The screening-level risk characterizations will inform EPA on the need for further work on individual chemicals or categories. Efforts are currently underway to consider how best to utilize these screening-level risk characterizations as part of a risk-based decision-making process on HPV chemicals which applies the results of the successful U.S. High Production Volume Challenge Program and the IUR to support judgments concerning the need, if any, for further action.

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[1] U.S. EPA. High Production Volume (HPV) Challenge Program; http://www.epa.gov/chemrtk/index.htm.
[2] U.S. EPA. HPV Challenge Program – Information Sources; http://www.epa.gov/chemrtk/pubs/general/guidocs.htm.
[3] U.S. EPA. HPV Chemicals Hazard Characterization website (http://www.epa.gov/hpvis/abouthc.html).
[4] U.S. EPA. Risk Assessment Guidelines; http://cfpub.epa.gov/ncea/raf/rafguid.cfm.
[5] OECD. Guidance on the Development and Use of Chemical Categories; http://www.oecd.org/dataoecd/60/47/1947509.pdf.
[6] U.S. EPA. Risk Characterization Program; http://www.epa.gov/osa/spc/2riskchr.htm.

SCREENING-LEVEL HAZARD CHARACTERIZATION
C_7 to C_9 Aliphatic Aldehydes and Carboxylic Acids Category

Introduction

The sponsor, Flavor and Fragrance High Production Volume Consortia, submitted a Test Plan and Robust Summaries to EPA for the C_6-C_{10} Aliphatic Aldehydes and Carboxylic Acids category (since changed to C_7-C_9 Aliphatic Aldehydes and Carboxylic Acids category) on May 2, 2001. EPA posted the submission on the ChemRTK HPV Challenge website on June 14, 2001 (http://www.epa.gov/chemrtk/pubs/summaries/alipalde/c13033tc.htm). EPA comments on the original submission were posted to the website on December 18, 2001. Public comments were also received and posted to the website. The sponsor submitted updated/revised documents on July 16, 2004 and February 4, 2005, which were posted to the ChemRTK website on September 20, 2004 and March 8, 2005, respectively. The C_7-C_9 aliphatic aldehydes and carboxylic acids category consists of the following chemicals:

Heptanal	CAS No. 111-71-7
Heptanoic Acid	CAS No. 111-14-8
Octanal	CAS No. 124-13-0
Nonanal	CAS No. 124-19-6

This screening-level hazard characterization is based primarily on the review of the test plan and robust summaries of studies submitted by the sponsor(s) under the HPV Challenge Program. In preparing the hazard characterization, EPA considered its own comments and public comments on the original submission as well as the sponsor's responses to comments and revisions made to the submission. Structure(s) of the sponsored chemical(s) and supporting chemical(s) is included in the appendix. The screening-level hazard characterization for environmental and human health toxicity is based largely on SIDS endpoints and is described according to established EPA or OECD effect level definitions and hazard assessment practices.

Category Justification

The four members of the C_7 to C_9 aliphatic aldehydes and carboxylic acids category are structurally similar 7-, 8- or 9-carbon aldehydes or carboxylic acids. The similarities in structure, physicochemical and environmental fate properties, environmental and mammalian toxicity and metabolism (*in vivo*, the aldehydes are rapidly converted to the corresponding carboxylic acids) allow these chemicals to be evaluated as a group, so that data for the tested category members can be used to provide estimates of similar properties for the untested members.

Supporting Chemical Justification

Supporting Chemical(s)	CAS No.	Endpoint(s) Supporting
2,6-Dimethyl-5-heptenal	106-72-9	Repeated-dose toxicity, reproductive toxicity, Carcinogenicity
Hexanal	66-25-1	Repeated-dose toxicity
Decanal	112-31-2	Acute toxicity to fish
Octanoic acid	124-07-2	Developmental toxicity
Nonanoic acid	112-05-0	Acute inhalation toxicity, repeated-dose toxicity, developmental toxicity

In their test plan, the sponsor supported the toxicity data for the category members with a number of additional studies for homologous aldehydes having fewer (hexanal) and more (decanal) carbons than the sponsored aldehydes and carboxylic acids corresponding to sponsored aldehydes (i.e. octanoic acid, nonanoic acid). EPA included these studies in the hazard evaluation. The sponsor used 2,6-dimethyl-5-heptenal, a branched aldehyde, as a supporting chemical for some health effects endpoints (repeated-dose and reproductive toxicity). EPA requested additional information on this chemical to demonstrate similarities between linear and branched aldehydes. The sponsor submitted information supporting the position that a 2-methyl substituent such as that in the proposed analog will not significantly change the overall metabolism of an aldehyde or carboxylic acid. The branched-chain substances

are oxidized to linear acid fragments that are similar or identical to those produced by the non-branched compounds. Thus, the use of the supporting chemical is adequately justified for the purposes of the HPV Challenge Program. The submitter's category analysis is available in its revised submission posted at the above-mentioned website.

Summary-Conclusion

The log K_{ow}s of the C_7 to C_9 aliphatic aldehydes and carboxylic acids category members indicate that their potential to bioaccumulate is expected to be low. Heptanal and heptanoic acid are readily biodegradable, indicating that they do not have the potential to persist in the environment. Nonanal is not readily biodegradable, indicating that it has the potential to persistent in the environment. No data were provided for octanal. Octanal is considered not readily biodegradable based on results from nonanal.

The evaluation of available aquatic toxicity data for fish, aquatic invertebrates and aquatic plants indicates that the potential acute hazard of the C_7 – C_9 aldehyde and carboxylic acid category members to aquatic organisms is moderate.

The acute toxicity of the category members is low by oral, dermal and inhalation routes of exposure. Repeated-dose studies revealed toxicity only at relatively high doses or exposure levels. The category members did not produce reproductive or developmental toxicity. They did not show mutagenic potential when evaluated in a variety of assays.

The potential health hazard of C_7-C_9 aldehydes and carboxylic acid category members is low based on repeated-dose, reproductive and developmental toxicity.

No data gaps have been identified under the HPV Challenge Program. All endpoints have been adequately addressed by a combination of test data and read across from appropriate category chemicals.

1. Physical-Chemical Properties and Environmental Fate

A summary of physical-chemical properties and environmental fate data submitted is provided in Table 1. For the purpose of the screening-level hazard characterization, the review and summary of these data was limited to the octanol-water partition coefficient and biodegradation endpoints as indictors of bioaccumulation and persistence, respectively.

Octanol-Water Partition Coefficient

Heptanoic acid (CAS No. 111-14-8)
Log K_{ow}: 2.4 (estimated)

Heptanal (CAS No. 111-71-7)
Log K_{ow}: 2.8 (measured)

Octanal (CAS No. 124-13-0)
Log K_{ow}: 3.5 (measured)

Nonanal (CAS No. 124-19-6)
Log K_{ow}: 3.3 (estimated)

Biodegradation

Heptanoic Acid (CAS No. 111-14-8)
(1) In a DOC die-away test, the inoculum was secondary effluent from unacclimatized activated sludge from the Frankfurt-Main plant. The test substance degraded 94.5% after 4 days.
Heptanoic acid is readily biodegradable.

Heptanal (CAS No. 111-71-7)
In a ready biodegradation test, heptanal was tested using inoculum that was the secondary effluent from an unacclimatized activated sludge from the Caterbury Sewage Works. Degradation was 74 and 53% after 28 days in duplicate tests. In another study, using the same inoculum, 63 and 74% degradation was noted in duplicate tests.
Heptanal is readily biodegradable.

Nonanal (CAS No. 124-19-6)
In a ready biodegradation test (manometric respirometry test) the inoculum was activated sludge. Degradation was 32% after 28 days.
Nonanal is not readily biodegradable.

Nonanoic acid (CAS No. 112-05-0, supporting chemical)
In a ready biodegradation test, nonanoic acid (a homolog for heptanoic acid) was tested in a modified Sturm test with activated sludge as the inoculum. The test substance degraded 72% after 29 days.
Nonanoic acid is readily biodegradable.

Conclusion: The log K_{ow}sof the C_7 to C_9 aliphatic aldehydes and carboxylic acids category members indicate that their potential to bioaccumulate is expected to be low. Heptanal and heptanoic acid are readily biodegradable, indicating that they do not have the potential to persist in the environment. Nonanal is not readily biodegradable, indicating that it has the potential to persistent in the environment. No data were provided for octanal. Octanal is considered not readily biodegradable based on results from nonanal.

Table 1. Summary of Physical-Chemical Properties and Environmental Fate Data

Endpoints	**Heptanoic acid (111-14-8)**	**Heptanal (111-71-7)**	**Octanal (124-13-0)**	**Nonanal (124-19-6)**
Melting Point (ºC)	**-8 (m)**	**-43 – -45 (m)**	No Data	No Data
Boiling Point Range (ºC)	**176 – 223 (m)**	**153[1]**	**163 – 173 (m)**	**154 – 191 (m)**
Vapor Pressure (hPa at 25°C)	0.01 – 0.15 (e)	4.7 (e)	0.8 – 23 (e)	0.53 – 0.75 (e)
Log K_{ow}	2.42 (e)	**2.8 (m)**	**3.5 (m)**	3.27 (e)
Water Solubility (mg/L at 25°C)	2419 (e)	2,274 (e)	715 (e)	132 (e)
Direct Photodegradation	No data Direct photolysis is not believed to contribute to degradation.			
Indirect (OH^-) Photodegradation $t_{1/2}$ (hr)	18.5 (e)	4.2 (e)	4.1 (e)	3.9 (e)
Stability in Water (Hydrolysis)	Stable in water and not subject to hydrolysis			
Fugacity (Level III Model)				
Air (%)	4.37	3.31	2.37	2.1
Water (%)	39.5	40.5	32.9	29.8
Soil (%)	56	56	64.5	67.6
Sediment (%)	0.147	0.132	0.256	0.491
Biodegradation at 28 days (%)	**94.5 (m) Readily biodegradable**	**53 – 74 (m) Readily biodegradable**	No data Not readily biodegradable (RA)	**32 (m) Not readily biodegradable**

(m) = measured data (i.e., derived from testing); (e) = estimated data (i.e. derived from modeling); (RA) = read-across;

2. Environmental Effects – Aquatic Toxicity

A summary of aquatic toxicity data submitted for SIDS endpoints is provided in Table 2. The table also indicates where data for tested category members are read-across (RA) to untested members of the category.

Acute Toxicity to Fish

Heptanoic Acid (CAS No. 111-14-8)
Fathead minnows (*Pimephales promelas*) were exposed to heptanoic acid for 96 hours at a nominal concentration of 120 mg/L in a semi-static system. Mean measured concentrations decreased during the test: 98% at 0 hours, 96% at 24 hours, 97% at 72 hours and 33%at 96 hours. The mean measured concentration was 92 mg/L. No mortalities or sublethal effects were observed throughout the exposure period.
96-h LC_{50} > 92 mg/L

Heptanal (CAS No. 111-71-7)
(1) Rainbow trout (*Salmo gairdneri;* 10 per concentration) were exposed to heptanal for 96 hours at concentrations of 0, 1, 3, 10, 30 or 10 mg/L. Mortality observed at 96 hours was: 0% at 0, 1 and mg/L; 10% at 10 mg/L and 100% at 30 and 100 mg/L.
96-h LC_{50} = 12 mg/L

(2) Guppies (*Poecilia reticulata;* 10 per concentration) were exposed to heptanal for 14 days under semi-static conditions.
14-d LC_{50} = 8.9 mg/L

Octanal (CAS No. 124-13-0)
(1) A 96-hour LC_{50} for fish, estimated by ECOSAR, was provided to support evaluation of the acute toxicity of octanal. The estimated concentration is consistent with the results obtained in the 14-day study with guppies.
96-h LC_{50} = 6.7 mg/L (estimated)

(2) Guppies (*P. reticulate*; 10 per concentration) were exposed to octanal for 14 days under semi-static conditions. Water concentrations were measured in the test, but were not provided in the robust summary.
14-d LC_{50} = 7.9 mg/L

Nonanal (CAS No. 124-19-6)
A 96-hour LC_{50} for fish estimated by ECOSAR was provided to support evaluation of the acute toxicity of nonanal. The estimated concentration is consistent with the results obtained in the 14-day study with guppies.
96-h LC_{50} = 4.8 mg/L (estimated)

Decanal (CAS No. 66-25-1, supporting chemical)
Guppy (*P. reticulate*; 10 per concentration) were exposed to decanal for 14 days under semi-static conditions. Water concentrations were measured in the test, but were not provided in the robust summary.
14-d LC_{50} = 3.10 mg/L

Acute Toxicity to Aquatic Invertebrates

Heptanoic Acid (CAS No. 111-14-8)
A 48-hour EC_{50} for *Daphnia*, estimated by ECOSAR, was provided to evaluate the acute toxicity of heptanoic acid.
48-h EC_{50} = 429 mg/L (estimated)

Heptanal (CAS No. 111-71-7)
(1) *Daphnia magna* (groups of 10) were exposed to heptanal at nominal concentration of 0, 2.6, 4.4, 7.2, 12 and 20 mg/L for 48 hours under flow-through conditions. Measured concentrations were 0, 1.9, 3.1, 5.1, 9.8 and 13.8 mg/L. Hazard characterization is based on this test because of flow-through conditions were employed and water concentrations were measured.
48-h EC_{50} = 4.13 mg/L

(2) *D. magna* (groups of 10) were exposed to heptanal at nominal concentration of 0, 1, 2, 5, 10, 20, 50, 100 and 200 mg/L for 48 hours under static conditions.
48-h EC_{50} = 54 mg/L

Octanal (CAS No. 124-13-0)
A 48-hour EC_{50} for *Daphnia*, estimated by ECOSAR, was provided to evaluate the acute toxicity of octanal.
48-h EC_{50} = 5.2 mg/L (estimated)

Nonanal (CAS No. 124-19-6)
D. magna (groups of 10) were exposed to nonanal at nominal concentration of 0, 0.7, 1.3, 2.2, 3.6 and 6.0 mg/L for 48 hours under flow-through conditions. Measured concentrations were 0, 0.32, 0.71, 1.12, 2.14 and 3.48 mg/L.
48-h EC_{50} = 1.54 mg/L

Toxicity to Aquatic Plants

Heptanoic Acid (CAS No. 111-14-8)
A 96-hour EC_{50} for green algae, estimated by ECOSAR, was provided to evaluate the acute toxicity of heptanoic acid.
96-h EC_{50} = 429 mg/L (estimated)

Heptanal (CAS No. 111-71-7)
(1) *Pseudokirchneriella subcapitata* were exposed to heptanal at nominal concentrations ranging from 0.1 to 50 mg/L for 96 hours.
96-h EC_{50} (growth) = 16 mg/L

(2) *P. subcapitata* were exposed to heptanal at nominal concentrations of 0, 3.3, 6.5, 13, 25, 50 and 100 mg/L for 72 hours. Measured concentrations were 0, 3.61, 6.47, 14.2, 25.7, 45.2 and 94.6 mg/L.
72-h EC_{50} (biomass) = 7.22 mg/L
72-h EC_{50} (growth) = 11 mg/L

Octanal (CAS No. 124-13-0)
A 96-hour EC_{50} for green algae, estimated by ECOSAR, was provided to evaluate the acute toxicity of octanal.
96-h EC_{50} = 17 mg/L (estimated)

Nonanal (CAS No. 124-19-6)
P. subcapitata were exposed to nonanal at nominal concentrations of 0, 0.25, 0.5, 1.0, 2.0, 4.0 and 8.0 mg/L for 72 hours. Mean measured concentrations were 0.196,0.453, 0.759, 1.47, 3.20 and 6.41 mg/L.
72-h EC_{50} (biomass) = 2.6 mg/L
72-h EC_{50} (growth) = 4.5 mg/L

Conclusion: The evaluation of available aquatic toxicity data for fish, aquatic invertebrates and aquatic plants indicates that the potential acute hazard of the C_7 – C_9 aldehyde and carboxylic acid category members to aquatic organisms is moderate.

Table 2. Summary of Environmental Effects – Aquatic Toxicity Data				
Endpoints	**Heptanoic acid (111-14-8)**	**Heptanal (111-71-7)**	**Octanal (124-13-0)**	**Nonanal (124-19-6)**
Fish **96-h LC_{50} (mg/L)** **14-day LC_{50} (mg/L)**	**> 92 (m)**	**12 (m)** **8.9 (m)**	6.7 (e) **7.9[1] (m)**	4.8 (e) **3.1[1] (m)**
Aquatic Invertebrates **48-h EC_{50} (mg/L)**	429 (e)	**4.1 - 54(m)**	5.2 (e)	**1.5 (m)**
Aquatic Plants **72-h EC_{50} (mg/L)** **(biomass)** **(growth)**	429 (e) (96-h)	**7.22(m)** **11 (m); 16 (m) (96-h)**	17 (e) (96-h)	**2.6 (m)** **4.5 (m)**

(m) = measured data (i.e., derived from testing); (e) = estimated data (i.e. derived from modeling); (RA) = Read Across;
[1]Data for decanal.

3. Human Health Effects

A summary of health effects data submitted for SIDS endpoints is provided in Table 3. The table also indicates where data for tested category members are read-across (RA) to untested members of the category.

Acute Oral Toxicity

Heptanal (CAS No. 111-71-7)
Rats (10) were administered a single oral dose of heptanoic acid at 5000 g/kg-bw and observed for 14 days. No deaths were reported. Clinical signs reported included lethargy and piloerection.
LD_{50} > 5000 mg/kg-bw

Heptanoic acid (CAS No. 111-14-8)
Albino rats (4/sex) were administered heptanoic acid at doses of 1350, 4556, 6834, 10,250 and 15,380 mg/kg-bw. Clinical symptoms included hypoactivity, salivation, labored breathing, muscular weakness and prostration.
LD_{50} = 8370 mg/kg-bw

Octanal (CAS No. 124-13-0)
Male Wistar rats (5) were administered octanal (mixed isomers) orally at 5.63 mL/kg-bw or 4616 mg/kg-bw. No additional details were provided in the robust summary.
LD_{50} = 4616 mg/kg-bw (mixed isomers)

Nonanal (CAS No. 124-19-6)
Sherman-Wistar albino rats (5/sex) were administered nonanal via gavage at 5000 mg/kg-bw and observed for 14 days. No deaths were reported.
LD_{50} > 5000 mg/kg-bw

Acute Dermal Toxicity

Heptanal (CAS No. 111-71-7)
Rabbits (10) were exposed dermally to a single dose of heptanal at 5000 mg/kg-bw. No deaths were reported. Clincial symptoms were skin irritation.
LD_{50} > 5000 mg/kg-bw

Heptanoic acid (CAS No. 111-14-8)
Albino rabbits (2/sex) were dermally exposed to undiluted heptanoic acid at 2000 mg/kg-bw and observed for 14 days. One mortality was reported. Severe erythema, edema, and second and third degree burns of the skin were reported at 24 hours, progressing to necrosis by 14 days.
LD_{50} > 5000 mg/kg-bw

Octanal (CAS No. 124-13-0)
Male New Zealand rabbits (4) were exposed dermally to octanal (mixed isomers) for 24 hours and observed for 14 days following the contact period.
LD_{50} = 5207 mg/kg-bw (mixed isomers)

Nonanal (CAS No. 124-19-6)
Albino rabbits (3 with intact skin; 3 with abraded skin) were exposed to a single dermal dose of nonanal at 5000 mg/kg-bw. Severe edema and burns were noted at the site of application.
LD_{50} > 5000 mg/kg-bw

Acute Inhalation Toxicity

Heptanal (CAS No. 111-71-7)
Sprague-Dawley rats (3/sex) were exposed to an atmosphere containing heptanal acid at a nominal concentration of 28 mg/L for 4 hours and observed for 14 days. Signs of irritation were noted during exposure and for several days post-exposure. Four animals died.
LC_{50} > 4700 mg/m^3 (4.7 mg/L)

Heptanoic acid (CAS No. 111-14-8)
Sprague-Dawley rats (5/sex) were exposed to an aerosol containing heptanoic acid at a nominal concentration of 5.9 mg/L for 4 hours and observed for 14 days. Signs of irritation were noted during exposure and for several days post-exposure. Four animals died.
LC_{50} > 4600 mg/m^3 (4.6 mg/L

Nonanoic acid (CAS No.112-5-0, supporting chemical)
Sprague-Dawley rats (5/sex) were exposed to an aerosol containing nonanoic acid at a nominal concentration of 5.9 mg/L for 4 hours and observed for 14 days. Signs of irritation were noted during exposure and for the first week post-exposure. Four animals died.
460 < LC_{50} < 3800 mg/m^3 (0.46 < LC_{50} < 3.8 mg/L)

Repeated-Dose Toxicity

Heptanoic Acid (CAS No. 111-14-8)
(1) Sprague-Dawley rats (10/sex/dose) were administered heptanoic acid via gavage at doses of 0, 875, 1750 or 3500 mg/kg-bw/day for 27 days. In the high dose group, several mortalities occurred in females and one death in males. Common clinical signs included lethargy, dyspnea, polypnea, tremors, wheezing, ataxia and excessive salivation. No changes were reported in clinical chemistry or hematology. High dose males showed decreased body weights and food consumption. Hyperkeratosis of the stomach was noted in high dose animals of both sexes. No treatment-related changes were noted at lower dose levels.
LOAEL = 3500 mg/kg-bw/day (based on body weight changes and stomach histopathology)
NOAEL = 1750 mg/kg-bw/day

(2) Heptanoic acid (500 mg/kg-bw) in mineral oil was applied to freshly clipped lateral and dorsal skin of New Zealand White rabbits (5/sex) daily, 5 days/week for 2 weeks. The skin of half of the animals was abraded prior to the first, sixth and eighth application. A control group was treated with mineral oil only. Following dosing, animals were allowed to recover for 2 weeks. After 2 weeks of treatment, six animals (three with abraded and three with intact skin) were necropsied and the remaining four animals were necropsied after an additional 2-week recovery period. Tissues from 29 organs were removed for microscopic evaluation. One death was recorded on day 11 of the study. Weight loss and severe local skin irritation (characterized by severe erythema and edema, necrosis and desquamation and exfoliation) were observed by the second week of exposure. Histopathology after 2 weeks

revealed hyperplasia, hyperkeratosis and necrosis of the skin at the application site. No other microscopic alterations were reported for any other tissue that could be related to administration of heptanoic acid. By the end of the 2-week recovery period, weight loss had disappeared and skin appeared healed.
LOAEL > 500 mg/kg-bw/day (highest dose tested)
NOAEL = 500 mg/kg-bw/day

Heptanal (CAS No. 111-71-7)
In a 28-day dermal toxicity test, heptanal (500 mg/kg-bw) in mineral oil was applied to freshly clipped lateral and dorsal skin of New Zealand White rabbits (5/sex) daily, 5 days/week for 2 weeks. The skin of half of the animals was abraded prior to the first, sixth and eighth application. A control group was treated with mineral oil only. After 2 weeks of treatment, six animals (three with abraded and three with intact skin) were necropsied and the remaining four animals were necropsied after an additional 2-week recovery period. Tissues from 29 organs were removed for microscopic evaluation. Most animals exhibited body weight loss after 1 or 2 weeks of treatment, but animals from the recovery group showed normal weight gain. Most animals showed local dermal irritation with slight to moderate erythema, localized necrosis and exfoliation. Histopathology revealed hyperplasia, hyperkeratosis and necrosis of the skin at the application site. No other microscopic alterations were reported for any other tissue that could be related to administration of heptanal. By the end of the 2-week recovery period, weight loss had disappeared and skin appeared healed.
LOAEL >500 mg/kg-bw/day (highest dose tested)
NOAEL = 500 mg/kg-bw/day

Nonanal (CAS No. 124-19-6)
(1) In a 28-day dermal toxicity test, nonanal (500 mg/kg-bw) in mineral oil was applied to freshly clipped lateral and dorsal skin of New Zealand White rabbits (5/sex) daily, 5 days/week for 2 weeks. The skin of half of the animals was abraded prior to the first, sixth and eighth application. A control group was treated with mineral oil only. After 2 weeks of treatment, six animals (three with abraded and three with intact skin) were necropsied and the remaining four animals were necropsied after an additional 2-week recovery period. Tissues from 29 organs were removed for microscopic evaluation. Most animals exhibited body weight loss after one or two weeks of treatment, but animals from the recovery group showed normal weight gain. Most animals showed local dermal irritation with slight to moderate erythema, localized necrosis and exfoliation. Histopathology revealed hyperplasia, hyperkeratosis and necrosis of the skin at the application site. No other microscopic alterations were reported for any other tissue that could be related to administration of nonanal. By the end of the 2-week recovery period, weight loss had disappeared and skin appeared healed.
LOAEL > 500 mg/kg-bw/day (highest dose tested)
NOAEL = 500 mg/kg-bw/day

Nonanoic acid (CAS No. 112-05-0, supporting chemical)
In a 28-day dermal toxicity test, the supporting chemical, nonanoic acid (500 mg/kg-bw) in mineral oil was applied to freshly clipped lateral and dorsal skin of New Zealand White rabbits (5/sex) daily, 5 days/week for 2 weeks. The skin of half of the animals was abraded prior to the first, sixth and eighth application. A control group was treated with mineral oil only. After 2 weeks of treatment, six animals (three with abraded and three with intact skin) were necropsied and the remaining four animals were necropsied after an additional 2-week recovery period. Tissues from 29 organs were removed for microscopic evaluation. Most animals exhibited body weight loss after one or two weeks of treatment, but animals from the recovery group showed normal weight gain. Most animals showed local dermal irritation with slight to moderate erythema, localized necrosis and exfoliation. Histopathology revealed hyperplasia, hyperkeratosis and necrosis of the skin at the application site. No other microscopic alterations were reported for any other tissue that could be related to administration of nonanoic acid. By the end of the 2-week recovery period, weight loss had disappeared and skin appeared healed.
LOAEL > 500 mg/kg-bw/day (highest dose tested)
NOAEL = 500 mg/kg-bw/day

2,6-Dimethylhept-5-en-1-al (CAS No. 106-72-9, supporting chemical)
(1) Wistar rats (15/sex/dose) were administered the supporting chemical, 2, 6-dimethylhept-5-en-1-al, at doses (calculated from food consumption rates) of 0, 9, 37 or 150 mg/kg-bw/day for 13 weeks. No adverse clinical signs were reported during the exposure period and no effect was noted on body weight or food/water intake. Urinalysis revealed a transient and slight decrease in renal urinary concentrating ability in the high-exposure group males during week 6 of exposure and females at week 14. Plasma glucose levels were elevated in the high-exposure group. Higher hemoglobin concentrations in the treated groups were considered spurious and not treatment-related by the study director. Histopathological examination of the kidney revealed no histopathology related to $alpha_{2u}$-globulin-mediated nephrotoxicity[1] and histology of other tissues was unremarkable.
LOAEL = 150 mg/kg-bw/day (based on renal effects)
NOAEL = 37 mg/kg-bw/day

(2) Sprague-Dawley rats (10/sex/dose) were administered the supporting chemical, 2,6-dimethylhept-5-en-1-al, via gavage at 0, 300, 1500 or 3000 mg/kg-bw/day for 29 days. In the high-dose group, four animals (one male and three females) died during treatment. High-dose males showed increased alkaline phosphatase and serum albumin while high-dose females showed only increased serum albumin. High-dose animals of both sexes had increased liver and kidney weights. In the liver, hypertrophy of the hepatocytes was seen in the centrilobular region indicative of adaptive enzyme induction rather than an adverse health effect. High-dose males showed increased severity of hyaline droplets in cells lining the kidney tubules, which may be indicative of $alpha_{2u}$-globulin induced renal nephropathy[1]. At 1500 mg/kg-bw/day, dose-related increases in total protein and albumin levels and histopathology of the liver and kidney were reported. At 300 mg/kg-bw-day, there were no significant findings related to treatment.
LOAEL = 1500 mg/kg-bw/day (based on liver and kidney weight changes with accompanying microscopic changes)
NOAEL = 300 mg/kg-bw/day

Hexanal (CAS# 66-25-1, supporting chemical)
Sprague-Dawley rats (10/sex/dose) were administered hexanal in drinking water at concentrations of 0, 1.0, 10, 100 or 1000 mg/L (equivalent to doses of 0, 0.1, 0.9, 8.6 or 96 mg/kg-bw/day) for 28 days. No adverse effects were seen on body weight change, food and water consumption, hematological and clinical chemistry parameters, organ weights, or gross and histopathological examination of tissues and organs. Sporadic observations of dilated kidney pelvis (one animal each in the 10 and 100 mg/L treatment groups) and hydronephrosis (one animal at 1000 mg/L) were not dose- or treatment-related.
LOAEL > 96 mg/kg-bw/day (highest dose tested)
NOAEL = 96 mg/kg-bw/day

Reproductive Toxicity

Heptanoic acid (CAS No. 111-14-8)
In a reproductive/developmental toxicity study, female Sprague-Dawley rats (10/group) were administered heptanoic acid via gavage (in corn oil) at doses of 0, 200, 1000 or 2000 mg/kg-bw/day for one week prior to a 7-day cohabitation period through gestation, parturition and a 4-day postpartum period. Mortality occurred in the high-dose group (3 of 10 rats) and mid-dose group (1 of 10 rats). In the 1000 and 2000 mg/kg-bw/day dose groups, significant increases in the incidence of rales ($p < 0.01$) and excess salivation ($p < 0.01$) were reported during pre-mating and gestation. High-dose females also exhibited lethargy, unkempt coats and labored breathing. In the high-dose group, food consumption was reduced throughout the study, average maternal body weights were decreased on days 10 – 16 of gestation and body weight gains were significantly ($p < 0.05$) reduced. The high-dose group showed reduced mating and fertility that were related to mortality. However, the duration of cohabitation and fertility and

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[1]The presence of nephropathy in association with the hyaline droplet accumulation in male rats suggests that the nephropathy in the males is occurring by an $alpha_{2u}$-globulin-mediated mechanism which is male rat-specific and not considered relevant to humans. EPA's Risk Assessment Forum has outlined the key events and the data that are necessary to demonstrate this mode of action ($Alpha_{2u}$-Globulin: Association with Chemically Induced Renal Toxicity and Neoplasia in the Rat, EPA/625/3-91/019F). One of the key events, $alpha_{2u}$-globulin accumulation, has not been demonstrated. Therefore, the nephropathy is assumed to be relevant to human health and it is concluded that a NOAEL for nephropathy in male rats was not established.

gestation indices were comparable to controls. Rats in the 200 mg/kg-bw/day dose group also showed clinical signs, including a significant increase ($p < 0.01$) in the incidence of respiratory rales during pre-mating and gestation but not during lactation. No effects were noted on implantations, length of gestation, proportion of dams delivering at least one live pup or pup viability. Pup weights were reduced on day 4 post parturition in the high-dose group. No malformations or gross lesions were seen in pups at any dose level.
LOAEL (systemic toxicity) = 200 mg/kg-bw/day (based on increased incidence of respiratory rales)
NOAEL (systemic toxicity) = Not established
LOAEL (reproductive toxicity) > 2000 mg/kg-bw/day (highest dose tested)
NOAEL (reproductive toxicity) = 2000 mg/kg-bw/day

2,6-Dimethyl-5-heptenal (CAS No. 106-72-9, supporting chemical)
In a one-generation reproductive toxicity study conducted with the supporting chemical, 2,6-dimethyl-5-heptenal, female Sprague-Dawley rats (10/dose level) were administered the chemical via gavage for 7 days prior to mating and 32 days thereafter at doses of 0, 300, 1500 or 3000 mg/kg-bw/day. At 3000 mg/kg-bw/day, 8 of 10 females were moribund or found dead early in the pre-mating phase. At 3000 and 1500 mg/kg-bw/day, the dams exhibited salivation and decreased activity during the pre-mating period. Body weights were decreased at the two highest doses during pre-mating and pregnancy. At 300 mg/kg-bw/day, food consumption and body weight were reduced only during the pre-mating period and were not considered adverse effects. Pregnancy rates and fertility were similar in control and treated dams. Pup viability and litter size was reduced at 1500 mg/kg-bw/day. Effects observed in the two dams that survived in the high-dose group (3000 mg/kg-bw/day) were not considered because of the small sample size. Treatment had no effects on pups from the 300 mg/kg-bw/day dose group.
LOAEL (systemic toxicity) = 1500 mg/kg-bw/day (based on decreased body weight)
NOAEL (systemic toxicity) = 300 mg/kg-bw/day
LOAEL (reproductive toxicity) = 1500 mg/kg-bw/day (based on decrease in pup viability and pup weight)
NOAEL (reproductive toxicity) = 300 mg/kg-bw/day

Developmental Toxicity

Heptanoic Acid (CAS No. 111-14-8)
(1) Pregnant females rats (22/group) were administered heptanoic acid by gavage at doses of 0 or 1000 mg/kg-bw/day from day 6 through 15 of gestation. Dams were sacrificed and necropsied on gestation day 20. No mortality, clinical signs or any other signs of toxicity were evident in the dams. One-third of fetuses were examined for visceral abnormalities and two-thirds were subjected to skeletal examination. No effects on pups were recorded.
LOAEL (maternal/developmental toxicity) > 1000 mg/kg-bw/day (highest dose tested)
NOAEL (maternal/developmental toxicity) = 1000 mg/kg-bw/day

(2) In the reproductive/developmental toxicity study described previously, heptanoic acid caused dam mortality in the high-dose (3 of 10 rats) and mid-dose (1 of 10 rats) groups. In the 1000 and 2000 mg/kg-bw/day dose groups, maternal toxicity was observed as a significant increases in the incidence of rales ($p < 0.01$) and excess salivation ($p < 0.01$) during pre-mating and gestation. High-dose females also exhibited lethargy, unkempt coats and labored breathing. In the high-dose group, food consumption was reduced throughout the study, average maternal body weights were decreased on days 10 – 16 of gestation and body weight gains were significantly ($p < 0.05$) reduced. The high-dose group showed reduced mating and fertility that were related to mortality. Duration of cohabitation and fertility and gestation indices were comparable to controls. Rats in the 200 mg/kg-bw/day dose group also showed clinical signs, including a significant increase ($p < 0.01$) in the incidence of respiratory rales during pre-mating and gestation but not during lactation. No effect on reproductive performance was observed at any dose level in this study. No effects were noted on implantations, length of gestation, proportion of dams delivering at least one live pup or pup viability. Pup weights were reduced on day 4 post parturition in the high-dose group. No malformations or gross lesions were seen in pups at any dose level.
LOAEL (maternal toxicity) = 200 mg/kg-bw/day (based on increase in the incidence of rales)
NOAEL (maternal toxicity) = Not established
LOAEL (developmental toxicity) = 2000 mg/kg-bw/day (based on decreased pup weights)
NOAEL (developmental toxicity) = 1000 mg/kg-bw/day

Octanoic acid (CAS No. 124-07-2, supporting chemical)
An abbreviated developmental toxicity study was conducted using the Chernoff/Kavlock assay in which no visceral or skeletal examinations of pups is performed. Female Sprague-Dawley rats were administered octanoic acid via gavage at doses of 0, 1125 or 1500 mg/kg-bw/day. At both doses, decreased body weight was observed in the dams and the number of live pups was decreased. No effects in either dams or pups were noted at 1125 mg/kg-bw/day.
LOAEL (maternal toxicity) = 1500 mg/kg-bw/day (based on decreased body weight)
NOAEL (maternal toxicity) = 1125 mg/kg-bw/day
LOAEL (developmental toxicity) = 1500 mg/kg-bw/day (based on decreased number of live pups)
NOAEL (developmental toxicity) = 1125 mg/kg-bw/day

Nonanoic acid (CAS No. 112-05-0, supporting chemical)
Pregnant female rats (22/group) were dosed with nonanoic acid at 0 or 1500 mg/kg-bw/day during days 6-15 of gestation. On Day 20 of gestation, females were sacrificed. One-third of fetuses were examined for visceral abnormalities and two-thirds were subjected to skeletal examination. There were no effects on mortality, clinical signs, body weight changes, food consumption, and gross pathology. No effects were seen on mean ovarian, uterine, litter size, pregnancy rates, corpora lutae, implantation sites, fetal viability, fetal weight, sex, gross pathology or visceral and skeletal examination.
NOAEL for maternal and developmental toxicity = 1500 mg/kg-bw/day
LOAEL > 1500 mg/kg-bw/day

Genetic Toxicity – Gene Mutation

In vitro
Heptanal (CAS No. 111-71-7)
(1) In four reverse mutation assays (Ames assay) with *Salmonella typhimurium* strains TA97, TA98, TA100, TA1535, TA1537 and TA1538 and concentrations ranging from 1 up to 3600µg/plate was conducted with and without metabolic activation. No reproducible or dose-related response over solvent was seen.
Heptanal was not mutagenic in these assays.

(2) Heptanal was tested for mutagenicity i*n vitro* in a mouse lymphoma forward mutation assay, with and without metabolic activation. Concentrations were 0.78 to 100 nL/mL without and 6.25 to 250 ng/mL with metabolic activation. Moderate to high toxicity was seen at all doses. No mutagenic activity was seen.
Heptanal was not mutagenic in this assay.

Heptanoic acid (CAS No. 111-14-8)
(1) In two reverse mutation assays (Ames assay) with heptanoic acid and one with its homologue, octanoic acid were conducted using *Salmonella typhimurium* strains TA98, TA100, TA1535 and TA1537 and TA1538 and concentrations up to 150,000 µg/plate with and without metabolic activation. No increase in reverse mutation was seen.
Heptanoic acid was not mutagenic in these assays.

(2) Heptanoic acid was tested for mutagenicity i*n vitro* in a mouse lymphoma forward mutation assay, with and without metabolic activation and concentrations up to 900 Mg/mL. No mutagenic activity was noted.
Heptanoic acid was not mutagenic in this assay.

Octanal (CAS No. 124-13-0)
In reverse mutation assay (Ames assay) with *Salmonella typhimurium* strains TA98, TA100, TA1535 and TA1537 and concentrations of 444 µg/plate was conducted with and without metabolic activation. There was no increase in frequency of reverse mutations with or without metabolic activation.
Octanal was not mutagenic in this assay.

Nonanal (CAS No. 124-19-6)
(1) In three reverse mutation assays (Ames assay) with nonanal and one with nonanoic acid were conducted using *Salmonella typhimurium* strains TA97, TA98, TA100, TA1535 and TA1537 and TA1538 and concentrations up to 1000 µg/plate (10,000 µg/plate for nonanoic acid) with and without metabolic activation. No increase in reverse mutation was seen.

Nonanal was not mutagenic in these assays.

(2) Nonanal was tested for mutagenicity i*n vitro* in a mouse lymphoma forward mutation assay, with and without metabolic activation. Nonanal yielded negative results without metabolic activation and produced weak mutagenic activity with metabolic activation, but only at concentrations that were cytotoxic.
Nonanal was not mutagenic in this assay.

Genetic Toxicity – Chromosomal Aberrations

In vitro
Nonanal (CAS No. 124-19-6)
(1) In five cytogenetic assays conducted in rat hepatocytes up to 16, 200 µg/plate, no increase in chromosomal aberrations or micromuclei was seen.
Nonanal did not induce chromosomal aberrations in these assays.

In vivo
Heptanal, 2,6-dimethyl-5-heptenal (CAS No. 106-72-9, supporting chemical)
In mouse micronucleus test, mice were treated with the test substance at 0, 420, 980, and 1540 mg/kg-bw once via intraperitoneal injection. Mice were euthanized 30hours after treatment and bone marrow smears wee prepared, stained and scored. No increase in the number of micronucleated polychromatic erythrocytes was seen. No mutagenic activity was detected.
Heptanal, 2,6-dimethyl-5-heptenal did not induce chromosomal aberrations in this assay.

Additional Information

Carcinogenicity

Heptanoic Acid (CAS No. 111-14-8)
In a mouse skin-painting bioassay, heptanoic acid was applied unoccluded to the clipped intrascapular skin of 50 C3H/HeJ male mice 2 times/week for 80 weeks. The study design included two negative controls (completely untreated and mineral oil treated) and one positive control (0.05% benzo(a)pyrene (BaP) in mineral oil). The focus of the study was to determine whether the test material could induce skin tumors (either benign papillomas or carcinomas) at the site of application. Three of 50 heptanoic acid treated mice developed benign tumors (latency 66 weeks). One squamous cell malignant carcinoma was reported in the untreated control group (0 tumors in mineral oil control). The positive BaP control group produced a typical high incidence of carcinomas with a short latency. Because no malignant tumors were produced in the treated group and because the low incidence of benign tumors (3/50) was within historical ranges for negative controls, it was concluded that heptanoic acid was not carcinogenic in this assay.

Conclusion: The acute toxicity of the category members is low by oral, dermal, and inhalation routes of exposure. Repeated-dose studies revealed toxicity only at relatively high doses or exposure levels. The category members and their analogs did not produce reproductive or developmental toxicity. They did not show mutagenic potential when evaluated in a variety of assays.

The potential health hazard of C_7-C_9 aldehydes and carboxylic acid category members is low based on repeated-dose, reproductive, developmental toxicity.

Table 3. Summary of Human Health Data				
Endpoints	**Heptanoic acid (111-14-8)**	**Heptanal (111-71-7)**	**Octanal (124-13-0)**	**Nonanal (124-19-6)**
Acute Oral Toxicity LD_{50} (mg/kg-bw)	**8370**	**> 5000**	**4616 (mixed isomers)**	**> 5000**
Acute Dermal Toxicity LD_{50} (mg/kg-bw)	**> 2000**	**> 5000**	**5207 (mixed isomers)**	**> 5000**
Acute Inhalation Toxicity LC_{50} (mg/m^3)	**> 4600**	**> 4700**	No data > 4700 (RA)	**460 < LC_{50} <3800[4]**
Genetic Toxicity - Gene Mutation *In vitro*	**Negative**	**Negative**	**Negative**	**Negative**
Genetic Toxicity - Chromosomal Aberrations *In vitro*	No Data Negative (RA)	**Negative[1]**	No Data Negative (RA)	**Negative**
Repeated-Dose Toxicity NOAEL/LOAEL (mg/kg-bw/day)	**LOAEL = 3500** **NOAEL = 1750** **NOAEL = 500**	**NOAEL = 500** **LOAEL = 150[1]** **NOAEL = 37[1]** **LOAEL = 150[1]** **NOAEL = 300[1]** **NOAEL = 96[2]**	No Data NOAEL = 500 (RA)	**NOAEL = 500** **NOAEL = 500[4]**
Reproductive Toxicity NOAEL/LOAEL (mg/kg-bw/day)		No Data	No Data	No Data
Systemic Toxicity	**LOAEL = 200** **NOAEL = Not established**	**LOAEL = 1500[1]** **NOAEL = 300[1]**		
Reproductive Toxicity	**LOAEL > 2000** **NOAEL = 2000**	**LOAEL = 1500[1]** **NOAEL = 300[1]**		
Developmental Toxicity NOAEL/LOAEL (mg/kg-bw/day)		No Data	No Data	No Data
Maternal Toxicity	**LOAEL = 200** **NOAEL = Not established**		**LOAEL = 1500[3]** **NOAEL = 1125[3]**	**LOAEL = Not established[4]** **NOAEL = 1000[4]**
Developmental Toxicity	**LOAEL = 2000** **NOAEL = 1000**		**LOAEL = 1500[3]** **NOAEL = 1125[3]**	**LOAEL = Not established[4]** **NOAEL = 1000[4]**
Carcinogenicity	Information available			

Measured data in bold text; (RA) = Read Across; [1]Supporting chemical data, 2, 6-dimethylheptenal: [2]Supporting chemical data, hexanal; [3]Supporting chemical data, octanoic acid; [4] Supporting chemical data, nonanoic acid

4. Hazard Identification

The log K_{ow}s of the C_7 to C_9 aliphatic aldehydes and carboxylic acids category members indicate that their potential to bioaccumulate is expected to be low. Heptanal and heptanoic acid are readily biodegradable, indicating that they do not have the potential to persist in the environment. Nonanal is not readily biodegradable, indicating that it has the potential to persistent in the environment. No data were provided for octanal. Octanal is considered not readily biodegradable based on results from nonanal.

The evaluation of available aquatic toxicity data for fish, aquatic invertebrates and aquatic plants indicates that the potential acute hazard of the C_7 – C_9 aldehyde and carboxylic acid category members to aquatic organisms is moderate.

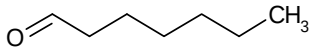
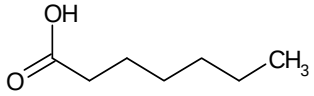
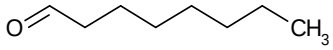
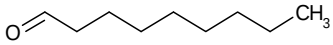
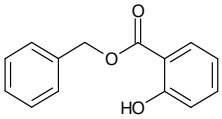
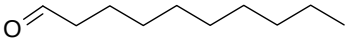
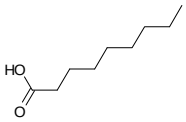
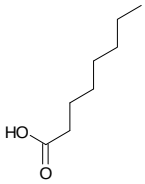
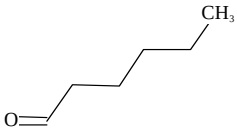
The acute toxicity of the category members is low by oral, dermal and inhalation routes of exposure. Repeated-dose studies revealed toxicity only at relatively high doses or exposure levels. The category members did not produce reproductive or developmental toxicity. They did not show mutagenic potential when evaluated in a variety of assays.

The potential health hazard of C_7-C_9 aldehydes and carboxylic acid category members is low based on repeated-dose, reproductive, developmental toxicity.

5. Data Gaps

No data gaps have been identified under the HPV Challenge Program. All endpoints required by the HPV Challenge Program have been adequately addressed by a combination of test data and read across from appropriate category chemicals.

Appendix

C_7 to C_9 Aliphatic Aldehydes and Carboxylic Acids Category		
CAS No.	**Chemical Name**	**Structure**
SPONSORED CHEMICALS		
111-71-7	**Heptanal**	 $C_7H_{14}O$
111-14-8	**Heptanoic Acid**	 $C_7H_{14}O_2$
124-13-0	**Octanal**	 $C_8H_{16}O$
124-19-6	**Nonanal**	 $C_9H_{18}O$
SUPPORTING CHEMICALS		
118-58-1	**Benzoic acid, 2-hydroxy-, phenylmethyl ester**	 $C_{14}H_{12}O_3$
112-31-2	**Decanal**	 $C_{10}H_{20}O$
112-05-0	**Nonanoic acid**	 $C_9H_{18}O_2$
124-07-2	**Octanoic acid**	 $C_8H_{16}O_2$
66-25-1	**Hexanal**	 $C_6H_{12}O$

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Keywords:	
Comments:	
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Change Number:	11
Last Saved On:	8/20/2007 3:27:00 PM
Last Saved By:	
Total Editing Time:	132 Minutes
Last Printed On:	8/20/2007 4:07:00 PM

As of Last Complete Printing

Number of Pages:	17
Number of Words:	7,311 (approx.)
Number of Characters:	41,161 (approx.)