The Flavor and Fragrance High Production Volume Consortia (FFHPVC)

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May 2, 2001

Christie Todd Whitman, Administrator
US EPA
P.O. Box 1473
Merrifield, VA 22116
Attn: Chemical Right-to-Know Program

Dear Ms. Whitman:

On behalf or the member companies of the C_6-C_{10} Consortium, the Flavor and Fragrance High Production Volume Consortia is pleased to submit the Test Plan and Robust Summaries for the chemical category designated the "C_6-C_{10} Aliphatic Aldehydes and Carboxylic Acids" to the HPV Challenge Program, AR-201. The C_6-C_{10} Consortium has chosen not to belong to the HPV Tracker System for submission of test plans and robust summaries. We are therefore submitting the test plan and accompanying robust summaries directly to EPA to make available to the public.

This submission includes one electronic copy in .pdf format. Hard copy can be provided upon request. The EPA registration number for the C_6-C_{10} Consortium is 1101124.

Please feel free to contact me with any questions or comments you might have concerning the submission at tadams@therobertsgroup.net, tadams@chemintox.com or 202-331-2325.

Sincerely,

Timothy Adams, Ph.D.
Technical Contact Person for FFHPVC

AR201-13033a

The Flavor and Fragrance High Production Volume Consortia

The C_6-C_{10} Consortium

Test Plan for C_6-C_{10} Aliphatic Aldehydes and Carboxylic Acids

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

FFHPVC C_6-C_{10} Aliphatic Aldehydes and Carboxylic Acids Consortium Registration Number

Submitted to the EPA under the HPV Challenge Program by:

The Flavor and Fragrance High Production Volume Chemical Consortia

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List of Member Companies

ATOFINA Chemicals, Inc.

Goodrich Corporation

Firmenich, Inc.

Celanese Corporation

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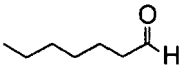
The HPV Challenge Test Plan for C_6-C_{10} Aliphatic Aldehydes and Carboxylic Acids

1 Identity of Substances



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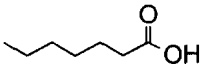

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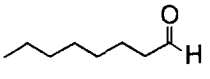

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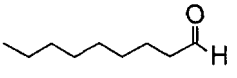


Nonanal
CAS No. 124-19-6

2 Category Analysis

2.1 Introduction

In October of 1999, members of the U.S. flavor and fragrance industries as well as other manufacturers that produce source materials used in flavors and fragrances formed consortia of companies in order to participate in the Chemical Right-to-Know Program. Members of these consortia are committed to assuring the human and environmental safety of substances used in flavor and fragrance products. The consortia are organized as the Flavor and Fragrance High Production Volume Consortia (FFHPVC). The C_6-C_{10} aliphatic aldehydes and carboxylic acids consortium, as a member of FFHPVC, serves as an industry consortium to coordinate testing activities for aliphatic substances under the Chemical Right-to-Know Program. Four (4) companies are current members of the C_6-C_{10} Consortium. The C_6-C_{10} Consortium and its member companies are committed to assembling and reviewing available test data, developing and providing test plans for each of the sponsored chemicals, and where needed, conducting additional testing. The test plan, category analysis and robust summaries presented represent the first phase of the Consortium's commitment to the Chemical Right-to-Know Program.

2.2 Background Information

This category analysis and test plan provides data for a group of three (3) saturated aliphatic acyclic linear aldehydes; heptanal, octanal, and nonanal, and one (1) carboxylic acid; heptanoic acid. The four substances in this chemical category are currently recognized by the U.S. Food and Drug Administration (FDA) as GRAS ("generally regarded as safe") for their intended use as flavoring substances [Hall and Oser, 1965]. Two aldehydes, octanal and nonanal, have been reviewed by the Joint Expert Committee on Food Additives (JECFA), a part of the World Health Organization (WHO) in 1984 at the twenty-eighth meeting of the Committee. The Committee established an acceptable daily intake (ADI) of 0.1 mg/kg bw/day for the combined use of octanal and nonanal based on the presumed *in vivo* oxidation to the corresponding acids and the results of a short-term study [JECFA, 1984].

By virtue of the fact that the aldehydes in this category are precursors of short-chain fatty acids or a short-chain fatty acid (heptanoic acid), they are expected to occur naturally in foods. Quantitative natural occurrence data indicate that oral intake of these substances occurs predominantly from consumption of food [Stofberg and Grundschober, 1987; Stofberg and Kirschman, 1985]. Greater than 1,000,000 kg of heptanal, octanal, and nonanal, and their corresponding carboxylic acids are consumed annually as natural components of traditional foods [Stofberg and Grundschober, 1987].

2.3 Structural Classification

The chemical category designated "C_6-C_{10} Straight Chain Aliphatic Aldehydes and Related Carboxylic Acids" includes a homologous series of straight chain saturated aldehydes of carbon chain length C_7 to C_9, heptanal, octanal, nonanal and one structurally related carboxylic acid, heptanoic acid. Heptanal is readily oxidized to heptanoic acid. The four substances are assigned to the same chemical category because of their close structural relationships and their similar physio-chemical properties. The three aldehydes are readily oxidized to their corresponding carboxylic acids in *vivo*. These carboxylic acids are endogenous in animals in that they are formed or broken down in the fatty acid pathway.

Heptanal and octanal are colorless liquids exhibiting a penetrating odor with a citrus-like aroma upon dilution. Nonanal is a colorless liquid with a fatty rose-like aroma. Heptanoic acid, better recognized as enanthic acid, is an oily liquid with a disagreeable, rancid, fatty odor that is faint when very pure [Bauer and Garbe, 1985].

2.4 Metabolism of Straight Chain Saturated Aliphatic Aldehydes and Carboxylic Acids

Linear aliphatic acyclic alcohols [DeBruin, 1976; Lington and Bevan, 1994], aldehydes [Brabec, 1993], and carboxylic acids [Katz and Guest, 1994; Dawson et *al., 1964;* von Oettingen, 1960] are absorbed through the gastrointestinal tract and are rapidly eliminated from the blood. Plasma half-lives are normally difficult to measure since many low molecular weight

aldehydes, and carboxylic acids (e.g., propionic acid) are endogenous in humans [Lington and Bevan, 1994]. Prior to absorption, simple aliphatic aldehydes may undergo oxidation to yield the corresponding carboxylic acid.

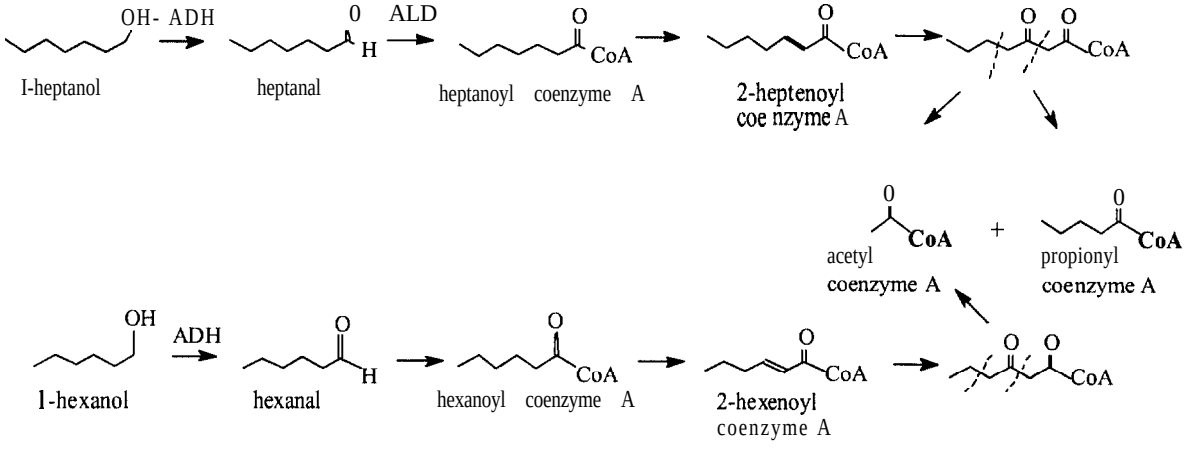
The primary metabolism of linear saturated aliphatic aldehydes and acids is a fundamental part of cell biochemistry. Aldehydes are successively oxidized to their corresponding carboxylic acids. The acid as the coenzyme A (CoA) ester then participates in the fatty acid pathway and the tricarboxylic acid cycle. To a minor extent, aldehydes also may be reduced to alcohols or conjugated with labile sulfhydryl-containing substances, such as glutathione [Brabec, 1993]. Medium chain carboxylic acids are condensed with acetyl CoA to form fatty acids (e.g., C_{10} to C_{18}) or undergo omega-oxidation to form diacids that are further metabolized by *beta*-oxidation in the fatty acid cycle [Katz and Guest, 1994].

A combination of high capacity dehydrogenase {alcohol (ADH) and aldehyde (ALD) dehydrogenase} and oxidase enzymes rapidly oxidize linear saturated aldehydes to the corresponding carboxylic acids (Figure 1). Most active is a NAD^+/NADH-dependent aldehyde dehydrogenase present in the cytosol that exhibits broad specificity for aliphatic and aromatic aldehydes [Feldman and Weiner, 1972]. It has been reported that the activity of this enzyme increases with increasing molecular weight of the aldehyde substrate [Nakayasu *et* al., 1978]. Molybdenum-containing enzymes, xanthine oxidase and aldehyde oxidase, also catalyze oxidation of a wide range of aldehydes to carboxylic acids [Levi and Hodgson, 1989].

The carboxylic acid resulting from oxidation of the aldehyde enters cellular fatty acid metabolism [Voet and Voet, 1990]. The acid is condensed with CoA to yield the corresponding thioester that undergoes dehydrogenation to form the *trans*-2-alkenoyl CoA (trans-Δ^2-enoyl CoA). The *trans*-Δ^2-alkenoyl CoA thioester is enzymatically converted to the S-3-hydroxy thioester and then to the 3-keto thioester. The thioester then undergoes beta-cleavage to yield an acetyl CoA fragment and a new thioester reduced by 2 carbons (Figure 1). Even numbered carbon acids (e.g. hexanoic or octanoic acid) continue to be cleaved to acetyl CoA while odd numbered carbon acids (e.g. pentanoic or heptanoic acid) yield acetyl CoA and propionyl CoA. Acetyl

CoA enters the citric acid cycle directly while propionyl CoA is methylated to R-methylmalonyl CoA, epimerized to the S isomer and finally isomerized to succinyl CoA *via the* action of methyhnalonyl CoA mutase. Succinyl CoA then enters the tricarboxylic acid cycle [Voet and Voet, 1990]. The high capacity species-specific enzymes that catalyze the reactions in these pathways result in rapid conversion of simple aliphatic aldehydes and carboxylic acids into carbon dioxide.

Figure 1. Metabolism of Aliphatic Primary Alcohols, Aldehydes and Carboxylic Acids



There is evidence of the complete metabolism of short-chain fatty acids. Twelve volunteers were given either l-l.5 mmole (2-3 μcurie/dose) of $^{14}C_1$-octanoic acid by oral administration or intravenous administration on separate occasions at least three days apart. Exhaled labeled carbon dioxide was first detected from l-2 minutes after intravenous administration and 2-6 minutes after oral administration. An average of 15.7% carbon dioxide was recovered within 50 minutes of oral or intravenous dosing [Schwabe *et al.*, 1964]. Based on this extensive biochemical data on the fatty acid pathway and citric acid cycle, the linear aliphatic aldehydes and acids in this chemical category are efficiently metabolized to carbon dioxide and water.

2.5 Summary for Category Analysis

Based on the known biochemical fate of straight chain aliphatic aldehydes and carboxylic acid, it is concluded that the aldehyde members of this chemical category undergo functional group oxidation to the corresponding carboxylic acid that is subsequently completely oxidized to carbon dioxide and water in the fatty acid pathway and tricarboxylic acid cycle. The physiochemical properties and low toxic potential of these substances are consistent with their known reactivity and common metabolic fate.

3 Test Plan

3.1 Chemical and Physical Properties

3.1.1 Melting Point

All the substances in this chemical category are liquids at ambient temperature. Calculated melting points for the lowest molecular weight aldehyde, heptanal, and heptanoic acid are 43.3 to 43.7 °C and -7.5 to -8 °C, respectively [Merck, 1997; Burdock, 1995; Arctander, 1969]. Given that the reported melting point for the structurally related homologous aldehyde pentanal is -91.5 °C [Hodgman *et* al., 1960], the melting points of octanal and nonanal are expected to be less than 0 "C.

3.1.2 Boiling Point

The three linear aliphatic aldehydes of this chemical category exhibit experimentally determined boiling points in the range from 152.6 to 191 °C at 760 mm Hg [Food Chemical Codex, 1996; Arctander, 1969; Merck, 1997; Burdock, 1995; Brabec, 1993]. The range of boiling points for linear aliphatic aldehydes having a chain length from C_5 to C_{10} is evenly distributed throughout the range of 103.4 to 207 °C [Hodgman et al., 1960].

While none of the reported boiling points was obtained according to currently recognized guidelines, the consistency of the values reported by five standard reference sources [Food Chemical Codex, 1996; Arctander, 1969; Merck, 1997; Burdock, 1995; Brabec, 1993] confirms their reliability. Likewise, the reported boiling point of 223 °C for heptanoic acid from three sources [Arctander, 1969; Hodgman *et al.,* 1960; Burdock, 1995] confii its reliability as does the fact that lower and higher homologues hexanoic acid (mp. 205.5 "C) and octanoic acid (mp. 239.3 "C) exhibit boiling points equally distributed below and above that for heptanoic acid [Hodgman *et al.,* 1960].

3.1.3 Vapor Pressure

The calculated vapor pressures for the three aliphatic aldehydes according to the MPBPWIN program range from 0.47 kPa (3.5 mm Hg) for heptanal, 0.21 kPa (1.6 mm Hg) for octanal, and 0.075 kPa (0.56 mm Hg) for nonanal at 25 "C. The calculated [FMA] or reported [Brabec, 1993] vapor pressures for heptanal (0.40 kPa or 3 mm Hg at 25 "C) and octanal (0.080 kPa or 0.6 mm Hg at 20 "C) are consistent with those calculated by MPBPWIN. Given the model and experimental data, the vapor pressures for the three aldehydes are in the range from 3.0 mm Hg (heptanal) to 0.05 mm Hg (nonanal). As anticipated, the MPBPWIN-calculated vapor pressure of 0.015 kPa (0.11 mm Hg) for heptanoic acid is significantly lower than the less polar corresponding aldehyde heptanal(0.47 kPa or 3.5 mm Hg).

3.1.4 Octanol/Water Partition Coefficients

The log Kow for heptanal measured by a reverse-phase HPLC method [Eadsforth, 1983] is 2.8, indicating a low potential for bioaccumulation from water. Calculated octanol/water partition coefficients have been determined by two methods [KOWIN and C-QSAR]. Predicted log Kow values for the three homologous aldehydes are from 2.29 for heptanal to 3.27 for nonanal [SRA]. The log Kow values of 2.42 for heptanal and 4.01 for nonanal predicted by C-QSAR [Nishimura, 1994] are consistent with calculated KOWIN values [SRA] and with the measured value of 2.8 for heptanal [Eadsforth, 1983]. The log Kow value of 2.42 for heptanoic acid [SRA] is consistent with that for its homologues, hexanoic acid (log Kow=2.05) and octanoic acid (log Kow=3.03) [SRC]. The log Kow value for heptanoic acid is expected to be lower than the measured Kow of 2.8 for the less polar substance heptanal. Based on these values, log Kow for the three aldehydes are in the range fi-om 2.5-4.0.

3.1.5 Water Solubility

Water solubilities of the four substances in this category have been determined by WSKOWIN. The calculated values for the three aldehydes are in the range from 2274 mg/L for heptanal to 132 mg/L for nonanal at 25 "C. The calculated solubility for heptanoic acid is 5316 mg/L at 25 °C [WSKOWIN] and is reported to be 242 mg/L at 15 °C [Merck, 1997].

3.1.6 New Testing Required

- Partition coefficient measurement for nonanal using an OECD Guideline HPLC reverse phase method to validate calculated values.

3.2 Environmental Fate and Pathways

3.2.1 Photodegradation

The calculated photodegradation half-lives for linear aliphatic aldehydes in this chemical category are in the narrow range from 3.9 hours for nonanal to 4.2 hours for heptanal [AOPWIN]. The half-lives for the aldehydes are shorter than those for the corresponding carboxylic acids. The half-lives for linear aliphatic carboxylic acids are in the range from 13.2 hours for nonanoic acid to18.5 hours for heptanoic acid [AOPWIN]. Generally, carboxylic acids are more stable to photolysis conditions than are the corresponding aldehydes. Structurally, the carboxyl free radical formed by hydrogen abstraction of a carboxylic acid is more stable than the enolic free radical formed by *the* &traction of *alpha* hydrogen of an aldehyde. The photodegradation half-lives of the aliphatic aldehydes and carboxylic acid in this category are estimated to be less than one day.

3.2.2 Stability In Water

None of the four substances in this chemical category are capable of hydrolysis. The volatilization half-lives calculated [HENRYWIN] for the three aldehydes are 5.0 to 5.9 hours for a model river and 5.1 to 5.2 days for a model lake. The volatilization half-lives calculated [HENRYWIN] for the three more polar corresponding carboxylic acids, heptanoic, octanoic, and nonanoic acids, are 14 to 25 days for a model river and 106 to 189 days for a model lake.

3.2.3 Biodegradation

Biodegradation tests have been performed for heptanal, nonanal, a homologous aldehyde, decanal, and a homologous acid, nonanoic acid. Heptanal undergoes ready biodegradation in both a closed bottle assay using an OECD 301D guideline [Watkinson, 1984] and in a modified Sturm test using an OECD 30 1B guideline [Watkinson, 1984]. Heptanal undergoes greater than

60% and 63-74% biodegradation after 10 and 28 days in a closed bottle assay and 53-74% biodegradation after 28 days in a modified Sturm test. Nonanal undergoes 50% and 84% biodegradation after 10 and 28 days, respectively using a OECD 302C protocol [Rudio, 1998a], but was only 29% and 32% biodegraded after 10 and 28 days, respectively, using an OECD 301F protocol [Rudio, 1994b]. Decanal was not ultimately biodegradable (i.e., 49.8%) in 28 days using an OECD 301B test protocol [Quest, 1995]. However, nonanoic acid was readily biodegradable. In a biodegradability test using an OECD 301B guideline, nonanoic acid was 72% biodegraded after 29 days [Comb, 1999]. Based on the data for the three linear aliphatic aldehydes and structurally related carboxylic acid nonanoic acid, it is concluded that the three aldehydes will be readily biodegradable as will heptanoic acid. However, in order to properly evaluate the results of the biodegradation study for short chain fatty acids, it is recommended that heptanoic acid be subjected to a biodegradability study according to a standard OECD protocol.

3.2.4 Fugacity

Transport and distribution in the environment were modeled using Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11 [Mackay, 1991]. The principal input parameters into the model are molecular weight, melting point, vapor pressure, water solubility, and log Kow. When measured values were available, they were used, but when they were not available, calculated data from the EPIWIN series of programs were used. Based on the similar structure and comparable physiochemical properties of the aliphatic aldehydes and carboxylic acids, it is not unexpected that these substances would exhibit similar distribution in the environment.

The model predicts that the three aldehydes are distributed mainly to the atmosphere (>80%). Consistent with water solubility and log Kow data the percentage (17%) of heptanal in water is greater than that for nonanal (5.3%) while nonanal, being more lipophilic, is found in higher percentage in the soil horizon (8.7% versus 2% for heptanal). The more polar substance, heptanoic acid is distributed mainly to the water (76.2%) and soil (17.7%). Based on this

physiochemical model, the ratio for distribution of the three aldehydes between water (2- 17%) and fish (0.00011 to 0.00049%) is greater than three orders of magnitude indicating low bioaccumulation.

The significance of these calculations must be evaluated in the context that the substances in this chemical category are products of plant and animal biosynthesis and are, therefore, ubiquitous in the environment. The model does not account for the influence of biogenic production on partitioning in the environment nor does it take into account the recognized reactivity (*i.e.*, oxidation) of linear aliphatic aldehydes. Therefore, the relevance of fugacity calculations for these substances must be evaluated in the context of these factors.

3.2.5 New Testing Required

- Biodegradability test for heptanoic acid using OECD Guideline 302B

3.3 Ecotoxicity

3.3.1 Acute Toxicity to Fish

A 14-day LC50 value *in Poecilia reticulata* has been reported for each of the three aldehydes in this chemical category [Deneer et *al.,* 1988]. An acute 96-hour LC50 has also been determined for heptanal *in Salmo gairdneri* [Stephenson, 1982]. Additionally, an acute 96-hr LC50 has been determined in juvenile fathead *minnows,* bleak, and *Nitocra spinipes* for each of the three corresponding alcohols, 1-heptanol, 1-octanol, and 1-nonanol [Broderius *et al.,* 1995; Bengtsson *et al.,* 1984]. The three alcohols are readily metabolized to the corresponding aldehydes in animals. ECOSAR calculated 96-hr LC50 values are normally less than measured values for the three aldehydes. A 96-hour LC50 has been reported for heptanoic acid [Bell, 1999].

In a semi-static assay in which test solutions were renewed daily, the 14-day LC50 in *Poecilia reticulata* was 8.8 mg/L for heptanal, 7.89 mg/L for octanal, and 3.10 for decanal [Deneer *et al.*, 1988]. The 96-hour LC50 of heptanal in Rainbow trout is reported to be 12 mg/L

[Stephenson, 1982]. These 14-day LC50 values are approximately the same as calculated 96-hour LC50 values of 8.8 mg/L for heptanal, 6.7 mg/L for octanal, and 4.8 mg/L for nonanal [ECOSAR].

The experimental 96-hour LC50 values for the corresponding alcohols are uniformly higher than those for the aldehydes. In juvenile fathead minnows, the 96-hour LC50 values increased from 37.9 mg/L for heptanol to 5.52 mg/L for nonanol [Broderius et *al.,* 1995]. In wild-caught bleak, 96-hour LC50 values decreased from 45 mg/L for heptanol to 16 mg/L for nonanol and, *in Nitocra spinipes,* the LC50 values decreased from 216 mg/L for heptanol to 25 mg/L for nonanol [Bengtsson *et al.,* 1984].

The calculated 96-hour LC50 value of 389 mg/L for heptanoic acid is almost two orders of magnitude greater than that calculated for heptanal [ECOSAR]. The experimental 96-hour LC50 of greater than 92 mg/L for heptanoic acid in fathead minnows [Bell, 1999] supports the high calculated LC50 for this simple organic acid. Based on 14-day and 96-hour LC50 studies for heptanal, octanal, and decanal and the series of aliphatic alcohols, the 96-hour LC50 values are anticipated to be greater than 10 mg/L, indicating that these aldehydes are of low acute toxic potential to fish. The corresponding acid, exhibiting a 96-hour LC50 approaching 100 mg/L, is even more innocuous. Given the current database of information, it will not be necessary to perform additional tests for this toxicity endpoint.

3.3.2 Acute Toxicity to Aquatic Invertebrates

An experimental 48-hour EC50 of 54 mg/L has been reported for *Daphnia magna* treated with heptanal [Stephenson, 1982]. The EC50 value is the concentration resulting in immobilization of 50% of the *Daphnia magna* after 48 hours. EC50 values would be expected to be less than measured LC50 values for heptanal. ECOSAR calculated LC50 values are available for all members of this chemical category. The calculated 96-hour LC50 values for fish and *Daphnia magna* are in the same order of magnitude (*i.* e., 1- 10 mg/L). For the three aldehydes, the 48-hour LC50 values are in the range from 4.8 mg/L for nonanal to 6.7 mg/L for heptanal. The calculated 48-hour LC50 values for the corresponding carboxylic acids are at

least an order of magnitude greater than the LC50 values for their corresponding aldehydes. The 4%hour LC50 values are in the range from 64 mg/L for nonanoic acid to 429 mg/L for heptanoic acid. The experimental data demonstrates that heptanal exhibits a low potential for toxicity to aquatic invertebrates. However, the QSAR algorithm should be validated by conducting an additional test on nonanal. Assuming the measured values for nonanal in *Daphnia magma* is greater than the calculated value, it will not be necessary to conduct this test on the homologue octanal or the oxidation metabolite of heptanal, heptanoic acid.

3.3.3 Acute Toxicity to Aquatic Plants

In a manner similar to invertebrate toxicity, an experimental EC50 value has been reported for heptanal. The 96-hour EC50 value for heptanal with *Selenastrum capricornutum* is 16 mg/L [Stephenson, 1982]. For the three aldehydes, the calculated 96-hour EC50 concentrations are in the range from 5.3 mg/L for nonanal to 44 mg/L for heptanal. The calculated 96-hour EC50 values for the corresponding carboxylic acids are up to two orders of magnitude greater than the EC50 values for their corresponding aldehydes. The 96-hour EC50 values are in the range from 44 mg/L for nonanoic acid to 429 mg/L for heptanoic acid. Given that experimental data is available only for heptanal, the QSAR algorithm should be validated by conducting an additional test on nonanal. Assuming the measured values for heptanal and nonanal in green algae are consistent and greater than calculated values, it will not be necessary to conduct this test on the homologue octanal or the oxidation metabolite of heptanal, heptanoic acid.

3.3.4 New Testing Required

- Acute toxicity to *Daphnia magna* by OECD guideline 202 for nonanal
- Acute toxicity to algae according to OECD guideline 201 for nonanal

3.4 Human Health Toxicity

3.4.1 Acute Toxicity

All substances in this category exhibit a very low order of acute oral and dermal toxicity in rats. Oral LD50 values for heptanal, octanal, and nonanal are all greater than 5000 mg/kg bw [Moreno, 1974, 1977; Shelanski, 1971; Smyth et *al.,* 1962; Harrison, 1976a]. Dermal LD50 values in the rabbit are also greater than 5000 mg/kg bw [Moreno, 1977; Shelanski, 197 1; Smyth et *al.,* 1962; Harrison, 1976b]. The inhalation LC50 for heptanal in rats is 4.7 mg/L [Berardi, 1989].

LD50 values by injection of 1200 and 600 mg/kg bw were reported for heptanoic and octanoic acid, respectively [Oro and Wretland, 1961]. Also for octanoic acid, oral LD50 values of 1283 mg/kg bw [Smyth *et al.,* 1962] and 10,080 mg/kg bw [Jenner et *al.,* 1964] have been reported in rats and a dermal LD50 value of greater than 5000 mg/kg bw [Moreno, 1977] has been reported in rabbits. The inhalation LC50 values for heptanoic and nonanoic acid in rats are 4.6 and 0.46-3.8 mg/L, respectively [Hoffman, 1990]. Based on the wealth of acute oral and dermal data, three aldehydes and heptanoic acid exhibit a low order of acute toxicity.

3.42 *In* vitro and *In vivo* Genotoxicity

As a group, saturated aliphatic acyclic linear aldehydes and carboxylic acids exhibited consistent negative results in the standard Ames assay (AMS), the unscheduled DNA synthesis test (UDS), cytogenetic assays, and mouse lymphoma assays. Following are separate discussions of the results of *in vitro* genotoxicity assays for aldehydes and carboxylic acids in this chemical category.

3.4.2.1 Heptanal, Octanal, and Nonanal

There was no evidence of mutagenicity for this homologous series of aliphatic aldehydes in studies using established strains of *Salmonella typhimurium (e.g.,* TA98, TA100, TA102, TA104, TA1535, TA1537, and TA1538) with or without S-9 metabolic activation [Jagannath,

1980; Mamett *et* al., 1985; Mortelmans *et* al., 1986; Florin *et al.,* 1980; Zeiger *et al.,* 1992]. Concentrations of up to 3333 µg/plate were used in standard [Florin *et al.,* 1980] and preincubation [Marnett *et al.,* 1985; Mortelmans *et al.,* 1986; Zeiger *et al.,* 1992] protocols. A variation on the standard Ames assay, which was also negative, used preincubation gene mutation induction with S-9 metabolic activation [Mortehnans *et al.,* 1986].

In mutation assays with mammalian cell lines, heptanal, which is negative in the Ames assay, also showed no evidence of an increase in the frequency of mutations when incubated with mouse lymphoma L5 178Y TK± (MLA) cells in the presence or absence of metabolic S-9 activation at concentrations up to 100 or 250 nl/ml, respectively. In the same assay, nonanal showed no evidence of mutagenicity at concentrations up to 25 nl/ml without metabolic activation and weak evidence of mutagenicity (2.2 times control values) with activation but only at cytotoxic concentrations (60 and 120 nl/ml) [Myhr, 198 1].

There was no evidence of unscheduled DNA synthesis when either rat or human hepatocytes were incubated with concentrations up to 100 mM nonanal [Martelli *et al.,* 1994].

In standard cytogenetic assays {i.e., chromosomal aberration (ABS) and sister chromatid exchange (SCE)}, no significant increase in ABS was reported when concentrations up to 100 uM (16,200 ug/plate) of nonanal were incubated with freshly prepared F344 rat hepatocytes [Esterbauer et al., 1990; Eckl et al., 1993]. There was no evidence of an increase in mitotic index or frequency of micronuclei when 16,200 ug/plate of nonanal was incubated with freshly prepared rat hepatocytes [Esterbauer *et* al., 1990; Eckl *et* al., 1993]. Nonanal induced a significant increase in the incidence of SCEs in rat hepatocytes but there was no dose-response relationship [Eckl *et al.,* 1993].

3.4.2.2 Heptanoic Acid and Homologues

There was no evidence of mutagenicity when 150,000 ug/plate of heptanoic acid and 50,000 ug/plate of octanoic acid were incubated using established *strains* of *Salmonella typhimurium* (e.g., TA98, TA100, TA1535, TA1537, and TA1538) with or without S-9 metabolic

activation [Heck et *al.*, 1989]. In the same strains, there was no evidence of mutagenicity for heptanoic acid with or without activation at concentrations up to 5000 or 10,000 ug/plate, respectively [San and Schadly, 1989] or for nonanoic acid with or without activation at 10,000 ug/plate [San and Kruel, 1989]. A modification of the standard Ames assay involving preincubation was also negative for a homologous series of 8 carboxylic acids (C_1, C_2, C_3, C_7, C_{10}, C_{12}, C_{14}, C_{18}) at concentrations of up to 10,000 &plate [Zeiger et *al.*, 1992].

In mutation assays with mammalian cell lines, heptanoic acid, which is negative in the Ames assay, exhibited a slight increase in the frequency of mutations when incubated with mouse lymphoma L5178Y TK± (MLA) cells in the presence of metabolic S-9 activation at concentrations greater than 600 ug/ml. The authors noted that culture conditions of low pH and high osmolality, which may occur upon incubation of mouse lymphoma cells with an acidic substance, have been shown to produce false-positive results in this and other assays. Therefore, they indicated that the results of this study should be interpreted cautiously [Heck et *al.*, 1989].

There was no evidence of unscheduled DNA synthesis when rat hepatocytes were incubated with concentrations up to 1000 nl/ml of heptanoic acid or 300 nl/ml of octanoic acid [Heck et *al.*, 1989].

In an *in vivo* assay with a structurally related heptenal derivative, there was no evidence of mutagenicity when *Drosophila melanogaster* were maintained on 25 mM of 2,6-dimethyl-5-heptenal for 3 days in a sex-linked recessive lethal assay [Wild *et al.*, 1983]. In a standard mouse micronucleus assay, there was no evidence of an increase frequency of micronuclei of bone marrow polychromatic erythrocytes when rats were given single intraperitoneal injections of up to 1540 mg/kg bw of 2,6-dimethyl-5-heptenal [Wild *et al.*, 1983].

3.4.2.3 Conclusions

Based on a weight of evidence approach, linear saturated aliphatic aldehydes and carboxylic acids *are* not mutagenic *in vitro* in the standard Ames assay, nor did they show evidence of

genotoxicity in standard UDS assays, or *in vitro* mutagenicity assays monitoring mitotic index, or in the incidence of micronuclei in rat hepatocytes. Results of assays in mouse lymphoma cells and cytogenetic assays such as ABS were predominantly negative. In addition, there was no evidence of *in vivo* genotoxicity for a structurally related aldehyde. Based on the above results and taking into account the endogenous nature of these substances and their known biochemical fate, it is concluded that the aliphatic linear aldehydes and carboxylic acids in this chemical category exhibit low genotoxic potential.

3.4.3 Repeat Dose Toxicity

3.4.3.1 *Octanal*

In an 86-day dietary study, rats (12/sex/group) were maintained on diets containing a mixture of aldehydes; G8: octanal (4 ppm), G9: nonanal (9 ppm), decanal: (2.2 ppm), undecanal (6 ppm), dodecanal and methyl nonyl acetaldehyde (8 ppm). The diet was calculated to provide an average daily intake of 112 mg/kg bw of aldehyde mixture for 12 weeks. Controls were maintained on an unsupplemented diet. After 12 weeks, urine samples were examined for presence of sugar and albumin, and blood was analyzed for hemoglobin levels. At necropsy, liver and kidney weights were measured and the liver and kidneys were subjected to histopathological examination. Based on measurement of growth, food intake, and efficiency of food utilization, hematological examination, urine analysis, liver and kidney weights, and histopathological examination of liver and kidney tissues, there was no evidence of toxicity associated with administration of the mixture of aldehydes [Trubek, 1958].

3.4.3.2 Heptanal and Heptanoic Acid

Groups (15/sex/dose) of Wistar rats were maintained on diets calculated to provide daily intakes of 0 (control), 9, 37 and 150 mg/kg bw/day of 2,6-dimethyl-5-heptenal for 13-14 weeks. Rats were examined daily for mortality and clinical signs. Water intake and body weight were recorded twice weekly. Food consumption was measured daily. Hematological examination *(i.e.,* hemoglobin concentration, erythrocyte count, packed cell volume and

leucocyte count), blood chemical determinations, and urine analysis (i.e., volume, pH, glucose, blood, bile, ketones and protein) were monitored at week 6 and at the end of the study, At termination, the rats were necropsied and histopathological examinations were performed on 26 tissues. At 150 mg/kg bw/day, a slight decrease in renal concentrating ability was reported at week 6 in males and at week 14 in females. Serum glucose levels of both sexes were elevated as compared to the controls at 150 mg/kg bw/day. The authors considered that the higher hemoglobin concentrations in treated groups were not adverse findings. The cause of the increased serum glucose level at the highest dose is unknown. There was no evidence of histopathology in any of the tissue examined including testes and ovaries. The authors considered the 37 mg/kg bw/day dietary level to be the no observable adverse effect level (NOAEL) [Gaunt *et al.,* 1983].

Groups (10/sex/group) of male and female Sprague-Dawley rats were given dose levels of 0, 300, 1500, or 3000 mg/kg bw of 2,6-dimethyl-5-heptenal [Terrill, 1990a] or 0, 875, 1750, or 3500 mg/kg bw of heptanoic acid [Terrill, 1990b] by gavage in corn oil (10 ml/kg) daily for 29 or 27 days, respectively. In both studies, clinical signs were monitored twice weekly and body weights and food consumption were measured weekly. At necropsy, blood was drawn and clinical chemistry, hematological determinations, and organ weights were measured. A variety of tissues (26) were prepared and preserved in 10% formalin. All tissues fi-om the control and high-dose groups and tissue fi-om the heart, liver, kidneys, and gross lesions from the low- and mid-dose group were embedded in paraffin, stained with hematoxylin and eosin, and examined microscopically.

Based on statistically significant changes in liver and kidney weights and histopathology of these organs at dose levels of 1500 and 3000 mg/kg bw/day, the lowest observable adverse effect level (LOAEL) and the no observable adverse effect level (NOAEL) for 2,6-dimethyl-5-heptenal were concluded to be 1500 and 300 mg/kg bw/day, respectively [Ten-ill, 1990a].

Based on decreased body weights and food consumption, gross lesions of the stomach, and microscopic lesions of the non-glandular region of the stomach at 3500 mg/kg bw/day, the

lowest observable adverse effect level (LOAEL) and the no observable adverse effect level (NOAEL) for heptanoic acid were concluded to be 3500 and 1750 mg/kg bw/day, respectively [Terrill, 1990b]. Except for tissue already discussed, there was no evidence of histopathology of other tissue including the testes and ovaries.

In a 28-day study, groups of SD rats (10/sex/group) were maintained on drinking water containing 1, 10, 100, or 1000 mg/L of hexanal for 4 weeks, Based on water intake data, the estimated average daily intake was 0.1, 0.9, 8.6, or 95.7 m&g bw. A control group received tap water and a vehicle control group received 0.5% Emuphor. Daily clinical observations and weekly measurements of body weight and food and water consumption revealed no significant difference between test and control animals. At termination, brain, heart, liver, spleen and kidneys weights showed no significant difference between test and control groups. Also at termination, hematological examination and clinical chemistry determinations showed normal values. Histopathology was performed on 26 tissues in controls and the highest exposure group revealed no microscopic alterations that could be associated with administration of the test material, No adverse effects were reported in this study [Komsta *et al.,* 1988].

In a 28-day dermal study, 500 mg/kg of heptanal, nonanal, heptanoic acid, or nonanoic acid in mineral oil (25% solution) was applied to the freshly clipped lateral and dorsal areas of groups of male and female New Zealand white rabbits (5/sex/group) daily for 5 days per week for 2 weeks. The skin of half the animals was abraded prior to the first, sixth, and eighth dose. A control group received mineral oil only. Viability was recorded twice daily, observations for skin irritation were made daily, and body weights were measured weekly. After 2 weeks, 6 animals (3 with abraided and 3 with intact skin) were necropsied with the remaining 4 animals sacrificed after an additional 2-week recovery period. Tissues from 29 organs were removed and preserved in 10% formalin. In all test groups, most animals exhibited a temporary weight loss after one or two weeks. Most animals treated with heptanal or nonanal showed slight to moderate erythema at the application site during the first week. Localized necrosis and exfoliation occurred in most animals during the second week. Microscopic evaluation revealed epidennal necrosis, epidermal hyperplasia, and hyperkeratosis at the application site. The skin

application sites of animals held to week 4 appeared healed. The sites were re-epithelialized and continuous with normal follicular structure and population. No other microscopic alterations were reported for any other tissue that could be related to administration of the test material [Auletta, 1981].

In an 80-week skin painting study, 50 mg of heptanoic acid was applied to the clipped backs of groups (50) of male C3H/HeJ mice. Negative control groups (50/group) were either untreated or treated with a mineral oil vehicle. A positive control group (50) was treated topically with 0.05% benzo(a)pyrene in mineral oil. Based on survival and body weight data, clinical observations, skin condition, and gross and histopathological examination, there was no evidence of significant toxicity or carcinogenicity in mice treated with heptanoic acid [Suskind, 1985].

Based on the NOAELs obtained in oral studies using an aldehyde structurally related to heptanal [Gaunt et *al.*, 1983; Ten-ill, 1990a], a mixture of linear aliphatic aldehydes [Trubek, 1958], heptanoic acid [Terrill, 1990b], and hexanal [Komsta *et al.*, 1988], it is concluded that the three aldehydes and heptanoic acid exhibit a low order of oral toxicity. The lowest NOAEL of 37 mg/kg bw/day is for an unsaturated aldehyde 2,6-dimethyl- 5-hetpenal that is anticipated to be more toxic than any aliphatic linear saturated aldehyde in this category. Data for hexanal, 2,6-dimethyl-5-heptanal in a second study, and the aldehyde mixture indicates that a NOAEL in excess of 300 mg/kg is expected for each aldehyde in the category. Heptanoic acid exhibits an even lower oral toxicity with a NOAEL exceeding 1000 mg/kg bw/day [Ten-ill, 1990b]. There is also low potential for dermal toxicity based on a dermal study using a 500 mg/kg bw/day dose level of heptanal, nonanal, heptanoic acid, or nonanoic acid for 28 days [Auletta, 198 1].

3.4.4 Reproductive Toxicity

A significant amount of data is derived from reproductive/developmental screening studies performed on heptanoic acid and a structurally related heptenal derivative. Although these studies do not meet OECD guideline standards for reproductive or developmental toxicity, they provide an extensive data set that in combination with the lack of histopathology in reproductive

organs of animals in repeat dose studies, indicate a low potential for reproductive or developmental toxicity.

Four groups of 10 virgin Crl CD rats were administered oral dose levels of 0, 200, 1000, or 2000 mg/kg bw of heptanoic acid or 0, 300, 1500, or 3000 mg/kg bw/day of 2,6-dimethyl-5-heptenal by gavage once daily, 7 days prior to cohabitation, through cohabitation (maximum of 7 days), gestation, delivery, and a 4-day post-parturition period. The duration of the study was 39 days [Vollmuth et al., 1995]. Maternal indices monitored included twice daily observation, measurement of body weights, food consumption, duration of gestation, and fertility parameters (mating and fertility index, gestation index, number of offspring per litter). Offspring indices included daily observation, clinical signs, examination for gross external malformations, and measurement of body weight.

In the heptenal study, clinical signs at 1500 and 3000 mg/kg in dams included significant ($P<0.05$ to <0.01) decreases in body weight and absolute and relative food consumption during the premating period. Eight rats of 10 in the high dose group were moribund or found dead on days 2, 3, and 4 of the premating period. Maternal body weights were decreased during gestation for the mid- and high-dose groups of dams.

Decreased body weights and absolute and relative food consumption in the 300 mg/kg bw/day group occurred only during premating and were not considered adverse effects. One of the two surviving high-dose dams delivered a litter that died during the 4-day lactation period. Mating and fertility at the high dose were similar to controls. Measurements of mating success and fertility were similar for controls, low-dose and mid-dose groups. Significant ($P<0.05$ to <0.01) decreases in pup viability occurred for mid-dose and high-dose groups as compared to controls. The mid-dose litters were significantly less ($P<0.05$) than control group litters. High-dose litters weighed markedly less than controls. No changes in averages for duration of cohabitation or gestation, inplantation sites or pup sex ratios were seen at any dose levels. No malformations or gross lesions in pups were attributable to administration of the test material. Based on the significant decrease in ($P<0.05$) pup weight at birth and pup viability in the mid-

dose group, the NOAEL for the F1 offspring was reported to be 300 mg/kg bw/day. The dose level of 300 mg/kg bw/day had no adverse effects on the reproductive performance of female Sprague-Dawley rats or the growth or development of their offspring [Vollmuth *et al.*, 1995].

In the heptanoic acid study, one and 3 deaths were reported in the 1000 and 2000 mg/kg bw/day dose groups, respectively. Clinical signs at 200 mg/kg bw/day in dams during premating and gestation included a significant increase in r-ales ($P<0.01$). This effect was not reported during the lactation period. In the 1000 and 2000 mg/kg bw/day dose group, significant increases in the incidence of rales ($P<0.01$), and excess salivation ($P<0.01$) were reported during premating and gestation. Excess salivation continued during lactation in the high-dose group. The 2000 mgikg bw/day group showed reduced body weight gains during premating, and significantly ($P<0.05$ to <0.01) decreased average maternal body weights on days 10 and 16 of gestation. Average and relative food consumption was reduced in the high-dose group of dams throughout the study. The high-dose was also associated with reduced mating and fertility that were related to mortality. The duration of cohabitation and fertility and gestation indices at 200, 1000, or 2000 mg/kg bw/day were not different from comparable indices in the control group. The high-dose group exhibited reduced pup weights on day 4 post-parturition. No biologically relevant or statistically significant differences in the number of implantations, duration of gestation, the percentage of dams delivering one or more live pups, and the pup viability index were observed. No malformations or gross lesions were observed in pups at any dose levels. The authors concluded that the dose level of 200 mgikg bw/day of heptanoic acid had no significant adverse effects on the reproductive performance of female Sprague-Dawley rats or the growth or development of their offspring [Vollmuth *et al.*, 1995].

Young female Wistar rats (10) were mated with males and the mating success was monitored by daily vaginal smears. Females were maintained on Purina Dog Chow and water ad libitum. Upon insemination, females were given daily oral doses of 2050 mg/kg bw/day of heptanal for 20 days. Body weights were measured daily and the difference in weight between the weight on the day of insemination, and immediately after parturition were also recorded. Based on the observation that there were no resorptions observed in any of the tested females, the authors

concluded that oral administration of 2050 mg/kg bw/day of heptanal resulted in no evidence of reproductive toxicity in female Wistar rats [Carruthers and Stowall, 1941].

3.4.5 Developmental/Teratogenicity Toxicity

Three linear aliphatic carboxylic acids were administered by gavage in corn oil to groups of pregnant Sprague-Dawley rats in a study designed to investigate the effect of aliphatic acid structure on developmental toxicity. Groups of rats received 100 or 133.3 mg butyric acid/kg bw, 75 or 100 mg pentanoic acid/kg bw, or 1125 or 1500 mg octanoic acid/kg bw daily by tracheal intubation on days 6 to 15 of gestation. Dams were allowed to deliver, and litters were examined through post-natal day 6. With varying degree, both dose levels of the three carboxylic acids resulted in an increase in mortality, a decrease in body weight gain and respiratory distress in treated females. With the exception of a significant decrease ($P<0.05$) in the number of live pups reported at the highest dose level (1500 mg/kg bw) with octanoic acid, there was no other evidence of fetotoxicity, developmental toxicity, or teratogenicity associated with administration of the three carboxylic acids [Narotsky et *al.*, 1994].

Pregnant NMRI mice (15/group) were given a single subcutaneous injection of 0 or 600 mg/kg bw of octanoic acid on day 8 of gestation. Dams were sacrificed on day 18 of gestation and examinations were performed for implantation sites. Each live fetus was individually weighed and inspected for the presence of neural tube defects. There was a non-statistically significant increase in embryolethality (15% in test group versus 7% in controls) and no effect of the test material on fetal weigh or on percentage of exencephaly in live fetuses. There was no evidence of embryotoxicity, teratogenicity, or fetal weight retardation [Nau and Loescher, 1986].

Xenopus embryos were collected following hormone-induced breeding. Each group of 25 embryos were exposed to a control, or 8 concentrations of heptanoic, octanoic, or nonanoic acid. Each acid was tested three times and data were pooled to calculate 96- hour LC50 (lethality), 96-hour EC50 (malformation), and to determine a development hazard index (DHI). For heptanoic, octanoic and nonanoic acids, the 96-hour LC50 values were 319.6, 127.1 and 32.7 mg/L, respectively; the 96-hour EC50 values were 51.3, 28.1, and 6.5 mg/L, respectively;

and the DHI was 6.2, 4.5 and 5.0. The authors noted that a DHI of less than 5.0 indicates a low developmental hazard while a value of greater than 5.0 indicates a moderate developmental hazard [Dawson *et al.,* 1996].

In an embryo/fetal toxicity and teratogenesis study, groups of 22 pregnant Sprague-Dawley rats were given 0 (corn oil vehicle), 1000 mg/kg bw of heptanoic acid, or 1500 mg/kg bw of nonanoic acid on days 6- 15 of pregnancy. Measurement of maternal body weights and food consumption and gross pathology revealed no evidence of maternal toxicity. Measurement of mean ovarian weight, uterine weight, litter size, pregnancy rates, corpora lutea, implantation sites, implantation efficiency, fetal viability, fetal size and sex, gross pathology, and visceral and skeletal examinations of fetuses revealed that there was no evidence of embryo toxicity, fetal toxicity, or teratogenesis related to administration of either heptanoic acid or nonanoic acid [Serota, 1983].

A single dose of 2700 mgikg bw of octanoic acid was administered to female Sprague-Dawley rats undiluted by oral gavage on the morning of day 12 of gestation (day0 = morning of finding vaginal plug). At day 20 of gestation, the rats were killed by chloroform overdose, and survivability, number of implantation sites, and mean fetal weight were recorded. Octanoic acid was devoid of embryotoxic effects except for a slight reduction of fetal weight that may be attributable to the severe maternal toxicity observed at the 2700 mg/kg dose [Scott *et al.*, 1994].

Based on the lack of histopathology of reproductive organs in repeat dose studies, the lack of significant reproductive or developmental effects in the absence of maternal toxicity in two reproductive/developmental screening studies, and the lack of developmental or fetotoxicity in studies with structurally related carboxylic acids, it is concluded that members of this chemical category show no significant evidence of either reproductive or developmental toxicity.

3.4.6 New Testing Required

None

3.5 Test Plan Table

Chemical	Physical-Chemical Properties				
	Melting Point	Boiling Point	Vapor Pressure	Partition Coefficient	Water Solubility
CAS No. 111-71-7 Heptanal	A	A, R	A, Calc	A, Calc	Calc
CAS No. 124-I 3-O Octanal	NA	A	Calc, R	Calc	Calc
CAS No. 124-19-6 Nonanal	NA	A, R	A, Calc	Test, Calc	Calc
CAS No. 111-14-8 Heptanoic acid	A	A, R	A, Calc	Calc	A, Calc

Chemical	Environmental Fate and Pathways			
	Photodegradation	Stability in Water	Biodegradation	Fugacity
CAS No. 111-71-7 Heptanal	Calc	Calc	A	Calc
CAS No. 124-I 3-O Octanal	Calc	Calc	R	Calc
CAS No. 124-I 9-6 Nonanal	Calc	Calc	A, R	Calc
CAS No. 11 l-l 4-8 Heptanoic acid	Calc	Calc	Test, R	Calc

Chemical	Ecotoxicity		
	Acute Toxicity to Fish	Acute Toxicity to Aquatic Invertebrates	Acute Toxicity to Aquatic Plants
CAS No. 111-71-7 Heptanal	A, Calc, R	A, Calc	A, Calc
CAS No. 124-13-O Octanal	A, Calc, R	R, Calc	R, Calc
CAS No. 124-19-6 Nonanal	Calc, R	Test, R, Calc	Test, R, Calc
CAS No. 111-14-8 Heptanoic acid	A, Calc	Calc	Calc

Chemical	Human Health Data					
	Acute Toxicity	Genetic Toxicity *In Vitro*	Genetic Toxicity *In Vivo*	Repeat Dose Toxicity	Repro-ductive Toxicity	Develop-mental Toxicity
CAS No. 111-71-7 Heptanal	A	A	R	A, R	A, R	R
CAS No. 124-13-O Octanal	A	A	R	R	R	R
CAS No. 124-19-6 Nonanal	A	A	R	A, R	R	R
CAS No. 111-14-8 Heptanoic acid	A	A	R	A	A	A, R

Legend

Symbol	Description
R	Endpoint requirement fulfilled using category approach, SAR
Test	Endpoint requirements to be fulfilled with testing
Calc	Endpoint requirement fulfilled based on calculated data
A	Endpoint requirement fulfilled with adequate existing data
NR	Not required per the OECD SIDS guidance
NA	Not applicable due to physical/chemical properties
0	Other

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The Flavor and Fragrance High Production Volume Consortia

The C_6-C_{10} Consortium

Robust Summaries for C_6-C_{10} Aliphatic Aldehydes and Carboxylic Acids

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**

FFHPVC C_6-C_{10} Aliphatic Aldehydes and Carboxylic Acids Consortium Registration Number 1101124

Submitted to the EPA under the HPV Challenge Program by:

The Flavor and Fragrance High Production Volume Chemical Consortia

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List of Member Companies

ATOFINA Chemicals, Inc.

Goodrich Corporation

Firmenich, Inc.

Celanese Corporation

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The Flavor and Fragrance High Production Volume Consortia Robust Summaries for C_6-C_{10} Aliphatic Aldehydes and Carboxylic Acids

The evaluation of the quality of the following data uses a systematic approach described by Klimisch [Klimisch *et al*., 1996]. Based on criteria relating to international testing standards for categorizing data reliability, four reliability categories have been established. The following categories are:

- Reliability code 1. Reliable without restrictions
- Reliability code 2. Reliable with restrictions
- Reliability code 3. Not reliable
- Reliability code 4. Not assignable

1 Chemical and Physical Properties

1.1 Melting Point

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.
Melting Point	-8 °C
Remarks for Results	The data are considered reliable.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Arctander S. (1969) Perfume and Flavor Chemicals (Aroma Chemicals) II. Published Montclair, NJ.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.

Melting Point	-45 °C
Remarks for Results	The data are considered reliable.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Brabec M. (1993) Aldehydes and Acetals in Patty's Industrial Hygiene and Toxicology 4th Ed., edited by G. Clayton and F. Clayton p. 286 John Wiley and Sons, Inc. New York, NY.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.
Melting Point	-43.7 °C
Remarks for Results	The data are considered reliable.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed. P 312, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.
Melting Point	-7.5 °C
Remarks for Results	The data are considered reliable.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed. P 314, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.
Melting Point	-7.5 °C
Remarks for Results	The data are considered reliable.

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Merck & Co., Inc. The Merck Index (1997) 12th Edition, Publishers: Merck Research Laboratories, Whitehouse Station, NJ.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.
Melting Point	-43.3 °C
Remarks for Results	The data are considered reliable.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Merck & Co., Inc. The Merck Index (1997) 12th Edition, Publishers: Merck Research Laboratories, Whitehouse Station, NJ.

Substance Name	Heptanal (data is for structurally related homologue pentanal)
CAS No.	111-71-7
Method/guideline	Measured
Remarks for Test Conditions	No test conditions provided.
Melting Point	-91.5 °C
Remarks for Results	The data are considered reliable.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co. Cleveland, Ohio.

1.2 Boiling Point

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Boiling Point	153 °C

Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Arctander S. (1969) Perfume and Flavor Chemicals (Aroma Chemicals) II. Published by the Author, Montclair, NJ.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Measured
Boiling Point	170 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Arctander S. (1969) Perfume and Flavor Chemicals (Aroma Chemicals) II. Published by the Author, Montclair, NJ.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Boiling Point	223 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Arctander S. (1969) Perfume and Flavor Chemicals (Aroma Chemicals) II. Published by the Author, Montclair, NJ.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Measured
Boiling Point	191 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Arctander S. (1969) Perfume and Flavor Chemicals (Aroma Chemicals) II. Published by the Author, Montclair, NJ.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Boiling Point	153 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Food Chemical Codex (1996) 4th Ed., National Academy Press, Washington, D.C.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Measured
Boiling Point	171 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Food Chemical Codex (1996) 4th Ed., National Academy Press, Washington, D.C.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Measured
Boiling Point	93 °C
Pressure	23 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Food Chemical Codex (1996) 4th Ed., National Academy Press, Washington, D.C.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Boiling Point	152.6 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed., CRC Press, Boca Raton, Fl.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Measured

Boiling Point	171- 173 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed., CRC Press, Boca Raton, Fl.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Boiling Point	223 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed., CRC Press, Boca Raton, Fl.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Boiling Point	115 - 116 °C
Pressure	11 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed., CRC Press, Boca Raton, Fl.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Measured
Boiling Point	191 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Burdock G. (1995) Fenaroli's Handbook of Flavor Ingredients. Volume II, 3rd Ed., CRC Press, Boca Raton, Fl.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Measured
Boiling Point	154 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Brabec M. (1993) Aldehydes and Acetals in Patty's Industrial Hygiene and Toxicology 4th Ed., Published by John Wiley and Sons, Inc. New York, NY.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Measured
Boiling Point	163.4 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg

Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Merck & Co., Inc. The Merck Index (1997) 12th Ed., Publishers: Merck Research Laboratories, Whitehouse Station, NJ.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Measured
Boiling Point	152.8 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Merck & Co., Inc. The Merck Index (1997) 12th Ed., Publishers: Merck Research Laboratories, Whitehouse Station, NJ.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Measured
Boiling Point	223 °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds, Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co., Cleveland, Ohio.

Substance Name	Heptanal (data on homologous aldehydes of carbon chain length of C5-C10)
CAS No.	111-71-7
Method/guideline	Measured
Boiling Point	103.4 (pentanal) °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds, Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co., Cleveland, Ohio.

Substance Name	Heptanal (data on homologous aldehydes of carbon chain length of C5-C10)
CAS No.	111-71-7
Method/guideline	Measured
Boiling Point	131 (hexanal) °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds, Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co., Cleveland, Ohio.

Substance Name	Nonanal (data on homologous aldehydes of carbon chain length of C5-C10)
CAS No.	124-19-6
Method/guideline	Measured

Boiling Point	207-209 (decanal) °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds, Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co., Cleveland, Ohio.

Substance Name	Heptanoic acid (data on structurally related acid, hexanoic acid)
CAS No.	111-14-8
Method/guideline	Measured
Boiling Point	205.5 (hexanoic acid) °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Reliabilities	The data are considered reliable.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds, Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co., Cleveland, Ohio.

Substance Name	Heptanoic acid (data on structurally related acid, octanoic acid)
CAS No.	111-14-8
Method/guideline	Measured
Boiling Point	239.3 (octanoic acid) °C
Pressure	760 mm Hg
Pressure Unit	mm Hg
Remarks for Results	No test conditions provided.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.

Remarks for Reliabilities	The data are considered reliable.
References	Hodgman C., Weast, R. C. and Selby, S. M. (1960) Tables for identification of organic compounds, Supplement to Handbook of Chemistry and Physics. Published by Chemical Rubber Publishing Co., Cleveland, Ohio.

1.3 Vapor Pressure

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Calculated
Vapor Pressure	0.053 kPa (0.4 mm Hg)
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are considered reliable.
References	Fragrance Materials Association (FMA)

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	MPBPWIN calculation
Vapor Pressure	0.47 kPa (3.5 mm Hg)
Temperature	25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	MPBPWIN

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	MPBPWIN calculation
Vapor Pressure	0.015 kPa (0.11 mm Hg)
Temperature	25 °C

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	MPBPWIN

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	MPBPWIN calculation
Vapor Pressure	0.21 kPa (1.6 mm Hg)
Temperature	25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	MPBPWIN

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	MPBPWIN calculation
Vapor Pressure	0.006 kPa (0.045 mm Hg)
Temperature	25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	MPBPWIN

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	MPBPWIN calculation
Vapor Pressure	0.075 kPa (0.56 mm Hg)
Temperature	25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.

References	MPBPWIN

Substance Name	Nonanoic acid
CAS No.	112-05-0
Method/guideline	MPBPWIN calculation
Vapor Pressure	0.0003 kPa (0.0022 mm Hg)
Temperature	25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	MPBPWIN

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	No test conditions provided.
Vapor Pressure	0.40 kPa (3 mm Hg)
Temperature	25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Data in tabular form published in standard reference text.
References	Brabec M. (1993) Aldehydes and Acetals in Patty's Industrial Hygiene and Toxicology 4th Ed., John Wiley and Sons, Inc. New York, NY.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Calculated
Vapor Pressure	0.080 kPa (0.6 mm Hg)
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are considered reliable.
References	Fragrance Materials Association (FMA)

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Calculated
Vapor Pressure	0.001 kPa (0.008 mm Hg)
Temperature	20 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are considered reliable.
References	Fragrance Materials Association (FMA)

1.4 Octanol/Water Partition Coefficients

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	KOWWIN
Log Pow	2.29
Data Qualities Reliabilities	Reliability Code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	Syracuse Research Corporation (SRC) Private communication to FMA.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	KOWWIN
Log Pow	2.42
Data Qualities Reliabilities	Reliability Code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	Syracuse Research Corporation (SRC) Private communication to FMA.

Substance Name	Octanal
CAS No.	124-13-0

Method/guideline	KOWWIN
Log Pow	2.78
Data Qualities Reliabilities	Reliability Code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	Syracuse Research Corporation (SRC) Private communication to FMA.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	KOWWIN
Log Pow	3.27
Data Qualities Reliabilities	Reliability Code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	Syracuse Research Corporation (SRC) Private communication to FMA.

Substance Name	Heptanal
CAS No.	118-58-1
Method/guideline	C-QSAR, Biobyte Corp.
Year	1994
Log Pow	2.42
Remarks for Results	Data presented in tabular form. Value consistent with log P values for 10 other linear aliphatic aldehydes.
Data Qualities Reliabilities	Reliability Code 2. Reliable with restrictions.
Remarks for Data Reliability	Data appeared in a peer-reviewed journal and are consistent with other model data.
References	Nishimura H., Saito S., Kishida F., and Matsuo, M. (1994) Analysis of acute toxicity (LD50 values) of organic chemicals to mammals by solubility parameter (delta). Acute oral toxicity to rats. Japan Journal of Industrial Health 36, 314-323.

Substance Name	Nonanal (data for structural homologue, decanal)
CAS No.	124-19-6
Method/guideline	C-QSAR, Biobyte Corp.
Year	1994

Log Pow	4.01
Remarks for Results	Data presented in tabular form. Value consistent with log P values for 10 other linear aliphatic aldehydes.
Data Qualities Reliabilities	Reliability Code 2. Reliable with restrictions.
Remarks for Data Reliability	Data appeared in a peer-reviewed journal and are consistent with other model data.
References	Nishimura H., Saito S., Kishida F., and Matsuo, M. (1994) Analysis of acute toxicity (LD50 values) of organic chemicals to mammals by solubility parameter (delta). Acute oral toxicity to rats. Japan Journal of Industrial Health 36, 314-323.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	n-Octanol/Water Partition Coefficient/Reverse Phase HPLC Method
Year	1983
Remarks for Test Conditions	The test material (1/mg/mL) in a mobile phase of methanol/water (3:1) was applied at a flow rate of 1 ml/min to a reverse phase C18-coated silica gel column fitted with a UV detector. Retention time was used to determine log Pow.
Log Pow	2.8
Remarks for Results	Measure at pH=6.7
Conclusion Remarks	HPLC Pow=2.8 and fragment-addition method Pow=2.4. Results indicate a low potential for bioaccumulation of heptanal from water.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Eadsforth C. V. (1983) Heptanal: Determination of n-octanol/water partition coefficient using a reverse-phase HPLC method. Shell Research Limited, Sittingbourne Research Centre. SBRG.83.112. Unpublished report.

1.5 Water Solubility

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	WSKOWWIN calculation
Value (mg/L) at Temperature	2274 mg/L at 25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.

References	WSKOWWIN

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	WSKOWWIN calculation
Value (mg/L) at Temperature	5316 mg/L at 25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	WSKOWWIN

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	WSKOWWIN calculation
Value (mg/L) at Temperature	715 mg/L at 25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	WSKOWWIN

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	WSKOWWIN calculation
Value (mg/L) at Temperature	132 mg/L at 25 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	WSKOWWIN

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Method was not described.

Value (mg/L) at Temperature	242 at 15 °C
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are considered reliable.
References	Merck & Co., Inc. The Merck Index (1997) Published by Merck Research Laboratories, 12th ed., Whitehouse Station, NJ.

2 Environmental Fate and Pathways

2.1 Photodegradation

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	4.2 hrs
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	AOPWIN

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	18.5 hrs
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	AOPWIN

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	4.1 hrs
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.

References	AOPWIN

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	15.4 hrs
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	AOPWIN

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	3.9 hrs
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	AOPWIN

Substance Name	Nonanoic acid
CAS No.	112-05-0
Method/guideline	Calculation
Test Type	AOPWIN
Halflife t1/2	13.2 hrs
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
References	AOPWIN

2.2 Stability in Water

Substance Name	Heptanal - No hydrolysis possible
CAS No.	111-71-7
Method/guideline	HENRYWIN
Test Type	SAR model
Halflife t1/2	Volatilization half-lives of 5.9 hours from model river, and 5.1 days from model lake.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	HENRYWIN

Substance Name	Heptanoic acid - No hydrolysis possible
CAS No.	111-14-8
Method/guideline	HENRYWIN
Test Type	SAR model
Halflife t1/2	Volatilization half-lives of 25 days from model river, and 189 days from model lake.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	HENRYWIN

Substance Name	Octanal - No hydrolysis possible
CAS No.	124-13-0
Method/guideline	HENRYWIN
Test Type	SAR model
Halflife t1/2	Volatilization half-lives of 5.4 hours from model river, and 5.1 days from model lake.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	HENRYWIN

Substance Name	Heptanoic acid (data for homologue, octanoic acid) - No hydrolysis possible
CAS No.	124-07-2
Method/guideline	HENRYWIN
Test Type	SAR model
Halflife t1/2	Volatilization half-lives of 19 days from model river, and 141 days from model lake.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	HENRYWIN

Substance Name	Nonanal - No hydrolysis possible
CAS No.	124-19-6
Method/guideline	HENRYWIN
Test Type	SAR model
Halflife t1/2	Volatilization half-lives of 5.0 hours from model river, and 5.2 days from model lake.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	HENRYWIN

Substance Name	Nonanoic acid - No hydrolysis possible
CAS No.	112-05-0
Method/guideline	HENRYWIN
Test Type	SAR model
Halflife t1/2	Volatilization half-lives of 14 days from model river, and 106 days from model lake.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized SAR method and are consistent with chemical structure.
References	HENRYWIN

2.3 Biodegradation

Substance Name	Nonanal (data for structurally related homologue, decanal)
CAS No.	124-19-6
Method/guideline	The sealed vessel test is a CO2 production test based on OECD Guideline 301 B(1).
Test Type	Sealed Vessel Test
GLP	Yes
Year	1995
Contact Time	28 days
Innoculum	Secondary effluent from an unacclimatized activated sludge plant at URL North.
Remarks for Test Conditions	The test is conducted in a 160 ml vessel containing 100 ml mineral salt medium inoculated with secondary effluent and the respective test or reference material. The sealed vessels are incubated at 17-20 C on a rotary shaker for 28 days.
Degradation % After Time	49.8% after 28 days
Results	49.8% (95% confidence interval 41.1-58.5%)
10 day Window Criteria	No
Conclusion Remarks	The test material was not ultimately biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was conducted in accordance with GLP and OECD guidelines.
Reference	Quest International Ltd. (1995) Biodegradability test of decanal in a sealed vessel test. Private communication to RIFM.

Substance Name	Nonanal (data for metabolite, nonanoic acid)
CAS No.	124-19-6
Method/guideline	Sealed vessel test: Modified Sturm test
Test Type	OECD 301B CO2 evolution
GLP	Yes
Year	1999
Contact Time	28 days
Innoculum	Nonanoic acid was added to two vessels containing mineral salts inoculated with activated sludge (10 mg C/L)

Remarks for Test Conditions	Test concentration: 10 mg/l organic carbon. Test temp: 20-24C
Degradation % After Time	72% at 29 days
Results	Nonanoic acid achieved 10% degradation by Day 2, 60% by Day 10, and 72% on Day 29.
Time required for 10% degradation	2 days
10 day Window Criteria	Yes
Total degradation	No
Conclusion Remarks	The test substance achieved the 60% pass level by Day 10. Nonanoic acid can, therefore, be considered to be readily biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was conducted in accordance with OECD 301B guidelines.
Reference	Comb H. (1999) Pelargonic acid- Assessment of ready biodegradability- modified Sturm test. CSD 025/992285. Unpublished report to FFHPVC.

Substance Name	Nonanal (98.5% pure)
CAS No.	124-19-6
Method/guideline	Manometric Respirometry Test/OECD Guideline Method No. 302C (1981)
Test Type	OECD 302C CO2 evolution/O^2 replacement
GLP	Yes
Year	1998
Contact Time	28 days
Innoculum	A known concentration of nonanal (30 mg/L) is stirred with fresh activated sludge from a waste water treatment plant in a closed flask for up to 28 days at 25 C.
Remarks for Test Conditions	The amount of O2 taken up during biodegradation measured as % of theoretical oxygen demand was determined by measuring the quantity of O2 required to maintain constant volume in the respirometer flask. Sodium benzoate (100 mg/L) was the reference substance.
Degradation % After Time	84% after 28 days
Results	Nonanal achieved 72% degradation by day 3 and 84% on day 29
Time required for 10% degradation	<1 days
10 day Window Criteria	Yes
Total degradation	No
Conclusion Remarks	The test substance (70%) achieved the 60% pass level by day 10. Nonanal can be considered to be inherently biodegradable.

Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	The study was conducted in accordance with OECD 302C guidelines.
Reference	Rudio J. (1998a) Inherent biodegradability of Aldehyde C9 Nonylic according to OECD Guideline No. 302C. Unpublished report to FFHPVC.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	The sealed vessel test is a CO2 production test based on OECD Guideline 301 B
Test Type	OECD 301 B Modified Sturm Test
GLP	Yes
Year	1984
Contact Time	28 days
Innoculum	Secondary effluent from an unacclimatized activated sludge plant from Canterbury Sewage Works
Remarks for Test Conditions	Duplicate tests were conducted in a Sturm vessel inoculated with secondary effluent and the respective test (20 mg/L) or reference material (sodium benzoate, 20 mg/L). Total CO2 evolved was measured on days 2, 4, 11, 17, 23, and 28 days.
Degradation % After Time	74 and 53% after 28 days
Results	64 and 45 % degradation after 11 days. 74 and 53% after 28 days (heptanal). 88 and 50% degradation after 28 days (sodium benzoate)
Time required for 10% degradation	2 days
10 day Window Criteria	Yes
Conclusion Remarks	The test material and standard were readily biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was conducted in accordance with GLP and OECD guideline.
Reference	Watkinson R. J. (1984) Heptanal: An assessment of ready biodegradability. SBGR 002. Shell Research Limited, Sittingbourne Research Centre. Unpublished report.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Closed Bottle Test/OECD test guideline 301D
Test Type	301D measured as % O2 demand

GLP	Yes
Year	1984
Contact Time	28 days
Innoculum	Secondary effluent from an unacclimatized activated sludge plant from Canterbury Sewage Works was incubated with 2 mg/L heptanal or 3 mg/L standard (sodium benzoate) for 28 days at 20.1 C. O2 concentration was measured on 0, 1, 15, and 28 days.
Degradation % After Time	63 and 74% after 28 days
Results	Biodegradability measured as % theoretical O2 demand: heptanal 63 and 74%; sodium benzoate, 61 and 69%
Time required for 10% degradation	<1 day
10 day Window Criteria	Yes
Conclusion Remarks	Heptanal and standard showed >50% biodegradation after 5 days
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	The study was conducted in accordance with OECD 301D guidelines.
Reference	Watkinson R. J. (1984) Heptanal: An assessment of ready biodegradability. SBGR 002. Shell Research Limited, Sittingbourne Research Centre. Unpublished report.

Substance Name	Nonanal (97%)
CAS No.	124-19-6
Method/guideline	Manometric Respirometry Test/OECD Guideline Method No. 302C (1981)
Test Type	OECD 302C CO2 evolution/O2 replacement
GLP	Yes
Year	1994
Contact Time	28 days
Innoculum	A known concentration of nonanal (100 mg/L) is stirred with fresh activated sludge (100 mg/L) from a waste water treatment plant in a closed flask for up to 28 days at 22 C.
Remarks for Test Conditions	The amount of O2 taken up during biodegradation measured as % of theoretical oxygen demand was determined by measuring the quantity of O2 required to maintain constant volume in the respirometer flask. Sodium benzoate (100 mg/L) was the reference substance.
Degradation % After Time	32% after 28 days
Results	Nonanal achieved 29% degradation by Day 3 and 32% on Day 29. The reference material aniline was 40% degraded after 7 days and 65% after 14 days. The test material with and without

	aniline was not toxic to the microorganisms at the test concentrations.
Time required for 10% degradation	1-2days
10 day Window Criteria	No
Total degradation	No
Conclusion Remarks	The test substance undergoes 29% biodegradation by Day 10 and 32% by Day 28 Nonanal should not be regarded as readily biodegradable in this test.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	The study was conducted in accordance with OECD 301F guidelines.
Reference	Rudio J. (1998b) Ready biodegradability of Aldehyde C9 Nonylic according to OECD Guideline No. 301F. Unpublished report to FFHPVC.

2.4 Fugacity

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Air-Water Partition Coefficient
Absorption coefficient	0.0094
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal

CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	2.6
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	5.2
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	16.2
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	6.6
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.

References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	12900
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Air
Estimated distribution and Media Concentration	80.8%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.

Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Water
Estimated distribution and Media Concentration	17.2%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Soil

Estimated distribution and Media Concentration	2.0%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Sediment
Estimated distribution and Media Concentration	0.045%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I

Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Suspended Sediment
Estimated distribution and Media Concentration	0.0014%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Fish
Estimated distribution and Media Concentration	0.00011%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanal
CAS No.	111-71-7
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model

Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Aerosol
Estimated distribution and Media Concentration	.000021%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Air-Water Partition Coefficient
Absorption coefficient	0.00015
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8

Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	5.18
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	10.4
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	32.4
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	13.2
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D.

	(1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	400000
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Air
Estimated Distribution and Media Concentration	5.64%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or

	metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Water
Estimated Distribution and Media Concentration	76.2%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Soil
Estimated Distribution and Media Concentration	17.7%

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Sediment
Estimated Distribution and Media Concentration	0.39%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP

Media	Suspended Sediment
Estimated Distribution and Media Concentration	0.012%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Fish
Estimated Distribution and Media Concentration	0.001%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay

Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Aerosol
Estimated Distribution and Media Concentration	0.00045%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Air-Water Partition Coefficient
Absorption coefficient	0.015
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs

Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Soil-Water Partition Coefficient
Absorption coefficient	8.8
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Sediment-Water Partition Coefficient
Absorption coefficient	17.6
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal

CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	54.9
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Fish-Water Partition Coefficient
Absorption coefficient	22.3
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	28800
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Air
Estimated Distribution and Media Concentration	84.3%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.

References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Water
Estimated Distribution and Media Concentration	11.2%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Soil
Estimated Distribution and Media Concentration	4.43%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.

Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Sediment
Estimated Distribution and Media Concentration	0.098%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Suspended Sediment

Estimated Distribution and Media Concentration	0.0031%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Fish
Estimated Distribution and Media Concentration	0.00025%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Octanal
CAS No.	124-13-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I

Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Aerosol
Estimated Distribution and Media Concentration	0.000049%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Air-Water Partition Coefficient
Absorption coefficient	0.00035
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model

Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Soil-Water Partition Coefficient
Absorption coefficient	16.4
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Sediment-Water Partition Coefficient
Absorption coefficient	32.7
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2

Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	102
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Fish-Water Partition Coefficient
Absorption coefficient	41.6
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	952000
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Air
Estimated Distribution and Media Concentration	13.5%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D.

	(1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Water
Estimated Distribution and Media Concentration	49.3%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Soil
Estimated Distribution and Media Concentration	36.3%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or

	metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Sediment
Estimated Distribution and Media Concentration	0.81%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Suspended Sediment
Estimated Distribution and Media Concentration	0.025%

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Fish
Estimated Distribution and Media Concentration	0.0021%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility

Media	Aerosol
Estimated Distribution and Media Concentration	0.00026%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Air-Water Partition Coefficient
Absorption coefficient	0.033
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay

Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Soil-Water Partition Coefficient
Absorption coefficient	36.6
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Sediment-Water Partition Coefficient
Absorption coefficient	73.3
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs

Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	229
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Fish-Water Partition Coefficient
Absorption coefficient	93.1
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal

CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	80000
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Air
Estimated Distribution and Media Concentration	85.8%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Water
Estimated Distribution and Media Concentration	5.27%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Soil
Estimated Distribution and Media Concentration	8.68%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.

References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Sediment
Estimated Distribution and Media Concentration	0.19%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Suspended Sediment
Estimated Distribution and Media Concentration	0.0060%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.

Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Fish
Estimated Distribution and Media Concentration	0.00049%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal
CAS No.	124-19-6
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, estimated VP, log Kow, MP, water solubility
Media	Aerosol

Estimated Distribution and Media Concentration	0.00014%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Air-Water Partition Coefficient
Absorption coefficient	0.000036
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I

Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Soil-Water Partition Coefficient
Absorption coefficient	51.8
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Sediment-Water Partition Coefficient
Absorption coefficient	104
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model

Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Suspended Sediment-Water Partition Coefficient
Absorption coefficient	324
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Fish-Water Partition Coefficient
Absorption coefficient	132
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0

Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Aerosol-Air Partition Coefficient
Absorption coefficient	18000000
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Air
Estimated Distribution and Media Concentration	0.54%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Water
Estimated Distribution and Media Concentration	29.4%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Soil
Estimated Distribution and Media Concentration	68.5%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D.

	(1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Sediment
Estimated Distribution and Media Concentration	1.52%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Suspended Sediment
Estimated Distribution and Media Concentration	0.048%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or

	metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Fish
Estimated Distribution and Media Concentration	0.0039%
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

Substance Name	Nonanal (Data for metabolite, nonanoic acid)
CAS No.	112-05-0
Model Conditions	25 °C, 100,000 lbs
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used	EQC V 2.11 Level I
Input Parameters	MW, VP, log Kow, water solubility, estimated MP
Media	Aerosol
Estimated Distribution and Media Concentration	0.00039%

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The data are obtained by a recognized fugacity calculation method. Data are considered reliable with restriction because this method does not allow for biodegradation or metabolism. Reliable with restriction because this method does not allow for biodegradation or metabolism.
References	Level 1 Fugacity-based Environmental Equilibrium Partitioning Model Version 2.11. Based on Mackay, D. (1991) Multimedia environmental models: The fugacity approach. Lewis Publications, CRC Press, Boca Raton, FL.

3 Ecotoxicity

3.1 Acute Toxicity to Fish

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Experimental: data calculated by logit transform.
Test Type	14 day LC50
GLP	No
Year	1988
Species/Strain/Supplier	P. reticulata, lab-reared
Analytical Monitoring	Gas chromatography
Exposure Period	14 days
Remarks for Test Conditions	Semi-static assay with 10 fish/concentration. Fish were acclimated to water for 12 days prior to experiment. Control fish were exposed to 72 uL/L acetone as a carrier solvent for the aldehydes. Oxygen content, pH, and concentration of test compound tested 4 times immediately before beginning of experiment and then after each renewal of test solution. Fish were fed daily. Water concentrations measured by gas chromatography. LC50s corrected for loss by evaporation.
Observations	Not reported
Conclusion Remarks	14-Day log LC50 = 1.89 umoles/L or 77.6 umoles/L or 8.85 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Complete detail on all test conditions. Data on 17 aliphatic aldehydes showed excellent correlation between log Kow and log LC50 (14-day).
Reference	Deneer J.W., Steinen, W. and Hermans, J.L.M. (1988) The acute toxicity of aldehydes to the guppy. Aquatic Toxicology, 12, 185-192.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Experimental: data calculated by logit transform.
Test Type	14 day LC50
GLP	No

Year	1995
Species/Strain/Supplier	P. reticulata, lab-reared
Analytical Monitoring	Gas chromatography
Exposure Period	14 days
Remarks for Test Conditions	Semi-static assay with 10 fish/concentration. Fish were acclimated to water for 12 days prior to the experiment. Control fish were exposed to 72 uL/L acetone as a carrier solvent for the aldehydes. Oxygen content, pH, and concentration of test compound tested four times immediately before beginning of the experiment and then after each renewal of test solution. Fish were fed daily. Water concentrations were measured by gas chromatography. LC50s corrected for loss by evaporation.
Observations	Not reported
Conclusion Remarks	Acute toxicity (14 day LC50) = 1.79 umoles/L or 61.7 umoles/L or 7.89 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Complete detail on all test conditions. Data on 17 aliphatic aldehydes showed excellent correlation between log Kow and log LC50 (14-day).
Reference	Deneer J.W., Steinen, W. and Hermans, J.L.M. (1988). The acute toxicity of aldehydes to the guppy. Aquatic Toxicology, 12, 185-192.

Substance Name	Heptanal (data for metabolic precursor, 1-heptanol)
CAS No.	111-71-7
Method/guideline	Calculated LC50, continuous flow-through system
Test Type	96 hr LC50
GLP	NG
Year	1995
Species/Strain/Supplier	Juvenile fathead minnows (Pimephales promelas)
Analytical Monitoring	HPLC and GC
Exposure Period	96 hrs
Remarks for Test Conditions	96 hour LC50 tests were performed with 26-34 day old juvenile fathead minnows. Test protocol was a continuous flow-through system according to Broderius and Kahl, 1985. Tests were carried out at 4 or 5 concentration. No solvent was required in these tests. One control (in duplicate) was used.
Observations	Not reported
Conclusion Remarks	96 hr LC50 = 37.9 mg/L

Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	US EPA Laboratory Study
Reference	Broderius S.J., Kahl, M.D. and Hoglund, M.D. (1995). Use of joint toxic response to define the primary mode of toxic action for diverse industrial organic chemicals. Environmental Toxicology and Chemistry, 14(9), 1591-1605.

Substance Name	Heptanal (data for metabolic precursor,1-heptanol dissolved in water)
CAS No.	111-71-7
Method/guideline	Calculated LC50/Static System
Test Type	96 hr LC50
GLP	NG
Year	1984
Species/Strain/Supplier	Bleak (Alburnus alburnus), caught in Baltic Sea
Analytical Monitoring	Not reported
Exposure Period	96 hrs
Remarks for Test Conditions	Wild-caught bleak were kept at least two weeks in storage tanks with a continuous flow of natural brackish water. Bleak were fed daily until one day prior to test. All tests were performed under static conditions with no aeration of the test aquaria. Tests were performed at 6 concentrations with 1 control group. Experiments were performed in duplicate with 10 bleak per aquarium at each concentration.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 45 mg/L (95% CI, 42-49 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Methodology described in detail and results were recorded in tabular form.
Reference	Bengtsson B. E., Renberg, L. and Tarkpea, M. (1984). Molecular structure and aquatic toxicity - an example with C1-C13 aliphatic alcohols. Chemosphere, 13(5/6), 613-622.

Substance Name	Octanal (data for metabolic precursor, 1-octanol dissolved in water/acetone)
CAS No.	124-13-0
Method/guideline	Calculated LC50/Static System
Test Type	96 hr LC50
GLP	NG

Year	1984
Species/Strain/Supplier	Bleak (Alburnus alburnus), caught in Baltic Sea
Analytical Monitoring	Not reported
Exposure Period	96 hrs
Remarks for Test Conditions	Wild-caught bleak were kept at least two weeks in storage tanks with a continuous flow of natural brackish water. Bleak were fed daily until one day prior to test. All tests were performed under static conditions with no aeration of the test aquaria. Tests were performed at 6 concentrations with 1 control group. Experiments were performed in duplicate with 10 bleak per aquarium at each concentration.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 16 mg/L (95% CI, 15-17 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Methodology described in detail and results were recorded in tabular form.
Reference	Bengtsson B. E., Renberg, L. and Tarkpea, M. (1984). Molecular structure and aquatic toxicity - an example with C1-C13 aliphatic alcohols. Chemosphere, 13(5/6), 613-622.

Substance Name	Octanal (data for metabolic precursor, 1-octanol)
CAS No.	124-13-0
Method/guideline	Calculated LC50/Continous flow-through system
Test Type	96 hr LC50
GLP	NG
Year	1984
Species/Strain/Supplier	Juvenile fathead minnows (Pimephales promelas)
Analytical Monitoring	HPLC and GC
Exposure Period	96 hrs
Remarks for Test Conditions	96 hour LC50 tests were performed with 26-34 day old juvenile fathead minnows. Test protocol was a continuous flow-through system. Tests were carried out at 4 or 5 concentration. No solvent was required in these tests. One control (in duplicate) was used.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 13.5 mg/L
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.

Data Reliability Remarks	US EPA Laboratory Study
Reference	Broderius S.J., Kahl, M.D. and. Hoglund, M.D (1995) Use of joint toxic response to define the primary mode of toxic action for diverse industrial organic chemicals. Environmental Toxicology and Chemistry, 14(9), 1591-1605

Substance Name	Heptanal (data for metabolic precursor, 1-heptanol dissolved in water)
CAS No.	111-71-7
Method/guideline	Calculated LC50/Static System
Test Type	96 hr LC50
GLP	NG
Year	1984
Species/Strain/Supplier	Nitocra spinipes (laboratory cultures)
Analytical Monitoring	Not reported
Exposure Period	96 hrs
Remarks for Test Conditions	Experiment was performed under static conditions. Nitocra spinipes were harvested from 3-6 week-old laboratory cultures; 2 times 10 harpacticoids were exposed to each concentration (at least 6 concentrations) in standard laboratory test tubes containing natural brackish water.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 210 mg/L (95% CI, 170-250 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Methodology described in detail and results were recorded in tabular form.
Reference	Bengtsson B. E., Renberg, L. and Tarkpea, M. (1984) Molecular structure and aquatic toxicity - an example with C1-C13 aliphatic alcohols. Chemosphere, 13(5/6), 613-622.

Substance Name	Nonanal (data for metabolic precursor,1-nonanol)
CAS No.	124-19-6
Method/guideline	Calculated LC50/Continous flow-through system
Test Type	96 hr LC50
GLP	NG
Year	1995
Species/Strain/Supplier	Juvenile fathead minnows (Pimephales promelas)

Analytical Monitoring	HPLC and GC
Exposure Period	96 hrs
Remarks for Test Conditions	96 hour LC50 tests were performed with 26-34 day old juvenile fathead minnows. Test protocol was a continuous flow-through system. Tests were carried out at 4 or 5 concentration. No solvent was required in these tests. One control (in duplicate) was used.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 5.52 mg/L
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	US EPA Laboratory Study
Reference	Broderius S.J., Kahl, M.D. and Hoglund, M.D. (1995) Use of joint toxic response to define the primary mode of toxic action for diverse industrial organic chemicals. Environmental Toxicology and Chemistry, 14(9), 1591-1605.

Substance Name	Octanal (data for metabolic precursor, 1-octanol dissolved in acetone/water)
CAS No.	124-13-0
Method/guideline	Calculated LC50/Static System
Test Type	96 hr LC50
GLP	NG
Year	1984
Species/Strain/Supplier	Nitocra spinipes (laboratory cultures)
Analytical Monitoring	Not reported
Exposure Period	96 hrs
Remarks for Test Conditions	Experiment was performed under static conditions. Nitocra spinipes were harvested from 3-6 week-old laboratory cultures; 2 times 10 harpacticoids were exposed to each concentration (at least 6 concentrations) in standard laboratory test tubes containing natural brackish water.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 58 mg/L (95% CI 53-64 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Methodology described in detail and results were recorded in tabular form.
Reference	Bengtsson B. E., Renberg, L. and Tarkpea, M. (1984) Molecular structure and aquatic toxicity - an example with C1-C13 aliphatic alcohols. Chemosphere, 13(5/6), 613-622.

Substance Name	Nonanal (data for metabolic precursor,1-nonanol dissolved in acetone/water)
CAS No.	124-19-6
Method/guideline	Calculated LC50/Static System
Test Type	96 hr LC50
GLP	NG
Year	1984
Species/Strain/Supplier	Nitocra spinipes (laboratory cultures)
Analytical Monitoring	Not reported
Exposure Period	96 hrs
Remarks for Test Conditions	Experiment was performed under static conditions. Nitocra spinipes were harvested from 3-6 week-old laboratory cultures; 2 times 10 harpacticoids were exposed to each concentration (at least 6 concentrations) in standard laboratory test tubes containing natural brackish water.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 25 mg/L (95% CI, 21-30mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Methodology described in detail and results were recorded in tabular form.
Reference	Bengtsson B. E., Renberg, L. and Tarkpea, M. (1984). Molecular structure and aquatic toxicity - an example with C1-C13 aliphatic alcohols. Chemosphere, 13(5/6), 613-622.

Substance Name	Nonanal (data for metabolic precursor, 1-nonanol dissolved in water/acetone)
CAS No.	124-19-6
Method/guideline	Calculated LC50/Static System Test
Test Type	96 hr LC50
GLP	NG
Year	1984
Species/Strain/Supplier	Bleak (Alburnus alburnus), caught in Baltic Sea
Analytical Monitoring	Not reported
Exposure Period	96 hrs
Remarks for Test Conditions	Wild-caught bleak were kept at least two weeks in storage tanks with a continuous flow of natural brackish water. Bleak

	were fed daily until one-day prior to test. All tests were performed under static conditions with no aeration of the test aquaria. Tests were performed at 6 concentrations with 1 control group. Experiments were performed in duplicate with 10 bleak per aquarium at each concentration.
Observations on Precipitation	Not reported
Conclusion Remarks	96 hr LC50 = 18 mg/L (95% CI, 16-20 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Methodology described in detail and results were recorded in tabular form.
Reference	Bengtsson B. E., L. Renberg and M. Tarkpea (1984). Molecular structure and aquatic toxicity - an example with C1-C13 aliphatic alcohols. Chemosphere, 13(5/6), 613-622.

Substance Name	Nonanal (data for homologous aldehyde, decanal)
CAS No.	124-19-6
Method/guideline	Experimental: data calculated by logit transform.
Test Type	14 day LC50
GLP	No
Year	1988
Species/Strain/Supplier	P. reticulata, lab-reared
Analytical Monitoring	Gas chromatography
Exposure Period	14 days
Remarks for Test Conditions	Semi-static assay with 10 fish/concentration. Fish were acclimated to water for 12 days prior to experiment. Control fish exposed to 72 uL/L acetone as a carrier solvent for the aldehydes. Oxygen content, pH, and concentration of test compound tested four times immediately before beginning of experiment and then after each renewal of test solution. Fish were fed daily. Water concentrations measured by gas chromatography. LC50s corrected for loss by evaporation.
Observations on Precipitation	Not reported
Conclusion Remarks	Acute toxicity (14 day LC50) = 1.31 umoles/L or 20.4 umoles/L or 3.10 mg/L. Note: 14-day LC50 data for octanal and decanal were determined to be 7.89 and 3.10 mg/L. It is anticipated that the 14-day LC50 is in the range of 3.10 to 7.89 mg/L.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	Complete detail on all test conditions. Data on 17 aliphatic aldehydes showed excellent correlation between lopKow and log LC50 (14-day).
Reference	Deneer J.W., Steinen, W. and Hermans, J.L.M. (1988) Acute toxicity of aldehydes to the guppy. Aqua. Tox. 12, 185-192.

Substance Name	Heptanoic acid (98.7%)
CAS No.	111-14-8
Method/guideline	Calculated LC50/Semi-static system
Test Type	96 hr LC50
GLP	Yes (OECD Guideline 203)
Year	1999
Species/Strain/Supplier	Juvenile fathead minnows/Aquatic Res. Organisms
Analytical Monitoring	HPLC
Exposure Period	96 hrs
Remarks for Test Conditions	96 hour LC50 tests were performed with 26-34 day old juvenile fathead minnows. Solutions were renewed daily during the 96 hour test period. Tests were performed at a nominal concentration of 120 mg/l. The mean measured concentration was 92 mg/L.
Observations on Precipitation	Not reported
Nominal concentrations as mg/L	120 mg/L
Measured concentrations as mg/L	92 mg/L
Remarks For Results	No mortalities or sub-lethal effects were throughout the exposure period. Mean measured concentrations were 98% at 0 hours, 96 and 97% at 24 and 72 hours, respectively and 33% at 92hours. The decrease in concentration at 92 hours was reported to be due to bacterial degradation of the test article.
Conclusion Remarks	96 hr LC50 > 92 mg/L
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliability Remarks	OECD Guideline 203 Study
Reference	Bell G. (1999) Heptanoic acid. Acute toxicity to fathead minnows (Pimephales promelas). Report No. CSD 017/992696. Unpublished report to FFHPVC.

Substance Name	Heptanal (98%, methyl hexanoate, 1%)
CAS No.	111-71-7
Method/guideline	Calculated LC50/Semi-static system
Test Type	96 hr LC50
GLP	No

Year	1982
Species/Strain/Supplier	*Salmo gairdneri* fingerlings/Itchen Valley Farm
Exposure Period	96 hrs
Remarks for Test Conditions	96 hour LC50 tests were performed with 10-day-old rainbow trout. Solutions were renewed daily. Groups of ten were exposed to 0, 1, 3, 10, 30, or 100 mg/L of heptanal. All groups received 0.5 ml acetone/L. Mortality was measured every 24 hours. The temperature during test was 15.1+/-1 C, pH=8.3+/-0.2, Dissolved oxygen=10.1+/-0.2 mg/L.
Nominal concentrations as mg/L	0, 1, 3, 10, 30, 100 mg/L
Remarks For Results	Mortality at 96 hours: 0 mg/L, 0/10; 1 mg/L, 0/10; 3 mg/L, 0/10; 10 mg/L, 1/10; 30 mg/L, 10/10; 100 mg/L, 10/10
Conclusion Remarks	96 hr LC50=12 mg/L(by log/probit method)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Reference	Stephenson R. R. (1982) Heptanal: Acute toxicity to salmo gairdneri, daphnia magna, and Selenastrum capricornutum. SBGR.82.197. Shell Research Limited, Sittinbourne Research Centre. Unpublished report.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	ECOSAR
Test Type	Calculated
Species/Strain/Supplier	Fish
Exposure Period	96 hrs
Conclusion Remarks	LC50 = 8.8 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	ECOSAR
Test Type	Calculated
Species/Strain/Supplier	Fish

Exposure Period	96 hrs
Conclusion Remarks	LC50 = 389 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	ECOSAR
Test Type	Calculated
Species/Strain/Supplier	Fish
Exposure Period	96 hrs
Conclusion Remarks	LC50 = 6.7 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	ECOSAR
Test Type	Calculated
Species/Strain/Supplier	Fish
Exposure Period	96 hrs
Conclusion Remarks	LC50 = 4.8 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

3.2 Acute Toxicity to Aquatic Invertebrates

Substance Name	Heptanal (98%, methyl hexanoate, 1%)
CAS No.	111-71-7
Method/guideline	48-Hour Static Toxicity Test
GLP	No
Year	1982
Species/Strain/Supplier	Daphnia magna
Unit	mg/L
Nominal concentrations as mg/L	0, 1,2, 5, 10, 20, 50, 100, 200 mg/L
Endpoint basis	Groups of 10 D. magna, less than 24 hours old, were allocated to a dish containing the heptanal conc. of 1.0 to 200 mg/L. All dishes received 0.5 ml acetone/L. At 24 and 48 hrs, the number of immobilized D magna were counted.
Biological observations	Immobiization test. D. magna were considered immobile, if after stirring they did not swim in 10 seconds.
EC50, EL50, LC0, at 24,48 hours	EC50 at 24 and 48 hours
Control response satisfactory?	Yes
Remarks for Test Conditions	Experiments were performed in triplicate at temperature of 20+/- 1 C, pH=8.0+/-0.2, hardness=210+/-20 mg/L as CaCO3, and dissolved oxygen=+9.1+/-0.1 mg/L.
Statistical evaluations	log/probit method
Remarks for Results	No immobilization at 0, 1, 2, or 5 mg/L. Cumulative total immobilised at 48 hours: 10 mg/L, 1/30; 20 mg/L, 3/30; 50 mg/L, 17/30; 100 mg/L, 20/30; 200 mg/L, 28/30. At 24 hours 200 mg/L, 10/30.
Conclusion Remarks	The 24 hr EC50>200 mg/L and 48 hr EC50=54 mg/L (95% C.I., 43-69 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Reference	Stephenson R. R. (1982) Heptanal:Acute toxicity to salmo gairdneri, daphnia magna, and Selenastrum capricornutum. SBGR.82.197. Shell Research Limited, Sittinbourne Research Centre. Unpublished Report.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Daphnid

Conclusion Remarks	LC50 48 hr = 6.7 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Daphnid
Conclusion Remarks	LC50 48 hr = 429 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Daphnid
Conclusion Remarks	LC50 48 hr = 5.2 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Octanal (data for oxidation metabolite, octanoic acid)
CAS No.	124-07-2
Method/guideline	ECOSAR
Test Type	Calculation

Species/Strain/Supplier	Daphnid
Conclusion Remarks	LC50 48 hr = 167 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Daphnid
Conclusion Remarks	LC50 48 hr = 4.8 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Nonanal (data for oxidation metabolite, nonanoic acid)
CAS No.	124-19-6
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Daphnid
Conclusion Remarks	LC50 48 hr = 64 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

3.3 Acute Toxicity to Aquatic Plants

Substance Name	Heptanal (98%, methyl hexanoate, 1%)
CAS No.	111-71-7
Method/guideline	96-Hour EC50 Growth Inhibition Assay
GLP	No
Year	1982
Species/Strain/Supplier	S. capricornutum/ATCC 22662/American Type Culture
Unit	mg/L
Nominal concentrations as mg/L	0, 0.1, 0.2, 0.5,1.0, 2.0, 5.0, 10, 20, and 50 mg/
Exposure period	96 hours
Endpoint basis	50% reduction in mean relative growth rate
Biological observations	Mean relative growth rate determined as the difference in log of noumber of cells at 48 and 96 hours/48 hours. EC50 value (conc. resulting in a 50% reduction in relative growth rate) determined by probit analysis.
Control response satisfactory?	Yes
Remarks for Test Conditions	In a 96-hr growth experiment, flasks containing 9 concentrations of heptanal were inoculated with S. capricornutum (500 cells/ml). Flasks were incubated in an orbital incubator at 24 C for 4 days. At 48 and 96 hrs cells were counted.
Statistical evaluations	Yes (probit analysis using log concentrations)
Conclusion Remarks	EC50 = 16 mg/L (95% C.I., 9.8-31 mg/L)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions
Reference	Stephenson R. R. (1982) Heptanal: Acute toxicity to salmo gairdneri, daphnia magna, and Selenastrum capricornutum. SBGR.82.197. Shell Research Limited, Sittinbourne Research Centre. Unpublished report.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Green algae

Exposure Period	96 hrs
Conclusion Remarks	EC50 = 44 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Green algae
Exposure Period	96 hrs
Conclusion Remarks	EC50 = 429 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Green algae
Exposure Period	96 hrs
Conclusion Remarks	EC50 = 17 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Octanal (data for oxidation metabolite, octanoic acid)
CAS No.	124-07-2
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Green algae
Exposure Period	96 hrs
Conclusion Remarks	EC50 = 110 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Green algae
Exposure Period	96 hrs
Conclusion Remarks	EC50 = 5.3 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

Substance Name	Nonanal (data for oxidation metabolite, nonanoic acid)
CAS No.	112-05-0
Method/guideline	ECOSAR
Test Type	Calculation
Species/Strain/Supplier	Green algae
Exposure Period	96 hrs

Conclusion Remarks	EC50 = 44 mg/l
Data Qualities Reliabilities	Reliability code 2. Reliability with restrictions.
Data Reliability Remarks	The data are obtained by a recognized SAR calculation and are consistent with chemical structure.
Reference	ECOSAR

4 Human Health Toxicity

4.1 Acute Toxicity

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	Oral LD50/calculated Litchfield and Wilcoxon, 1949
Test Type	Oral LD50
GLP	No
Year	1964
Species/strain	Rat/Osborne-Mendel
Sex	Male and Female
# of animals per sex per dose	10
Vehicle	No vehicle required
Route of Administration	Oral
Remarks for Test Conditions	Rats fasted for 18 hours prior to treatment. All doses were given by intubation and animals were observed for an additional 14 days.
Value LD50 or LC50 with confidence limits	Oral LD50 = 10,080 (8190-12370) (95% C.I.)
Number of deaths at each dose level	Death time reported at 4 hours to 9 days.
Remarks for Results	Clinical signs included depression and diarrhea.
Conclusion Remarks	Acute oral LD50 = 10080 (8190-12370) (95% C.I.)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Jenner P.M., E. C. Hagan, J.M. Taylor, E.L. Cook and O.G. Fitzhugh (1964) Food flavourings and compounds of related structure. I. Acute oral toxicity. Food Cosmetic. Toxicology. 2:327-343.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Oral LD50
Test Type	Oral LD50

GLP	No
Year	1974
Species/strain	Rat
Sex	Not reported
# of animals per sex per dose	10
Vehicle	None reported
Route of Administration	Oral
Remarks for Test Conditions	Animals given single oral dose of 5 g/kg and observed for 14 days.
Value LD50 or LC50 with confidence limits	LD50 > 5000 mg/kg (no confidence limits reported)
Number of deaths at each dose level	No deaths reported.
Remarks for Results	Clinical signs reported included lethargy and piloerection.
Conclusion Remarks	Oral LD50 > 5000 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Single dose to 10 animals.
References	Moreno O.M. (1974) Acute toxicity studies. Unpublished report to RIFM.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Oral LD50
Test Type	Oral LD50
GLP	No
Year	1971
Species/strain	Rat/Sherman-Wistar albino
Sex	Male and Female
# of animals per sex per dose	5
Vehicle	Not reported
Route of Administration	Oral (gavage)
Remarks for Test Conditions	Animals were fasted for 24 hours, then given single dose of 5 g/kg bw by gavage. Animals were given food and water ad libidum during a 14-day observation.

Value LD50 or LC50 with confidence limits	LD50 > 5000 mg/kg
Number of deaths at each dose level	No deaths reported.
Remarks for Results	Diuresis noted soon after dosing followed by lethargy and dullness. Recovery was complete 24-48 hr after dosing.
Conclusion Remarks	Oral LD50 > 5000 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Single dose to 10 animals.
References	Shelanski, M.V. (1971) Acute toxicity studies in rats. Unpublished report to RIFM.

Substance Name	Octanal (mixed isomers)
CAS No.	124-13-0
Method/guideline	Oral LD50
Test Type	Oral LD50
GLP	No
Year	1962
Species/strain	Rat/Wistar
Sex	Male
# of animals per sex per dose	5
Vehicle	Not specified
Route of Administration	Oral (gavage)
Remarks for Test Conditions	Five non-fasted male rats were used in this study. Chemicals administered undiluted (if possible) or diluted in water, corn oil or 1% TERGITOL via gastro-intubation.
Value LD50 or LC50 with confidence limits	5.63 mL/kg or 4616 mg/kg
Number of deaths at each dose level	No specifics reported.
Remarks for Results	No range was calculable because no dosage resulted in fractional mortality.
Conclusion Remarks	Oral LD50 = 5.63 mL/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	No details regarding doses and mortality.
References	Smyth Jr., H.F., C. P. Carpenter, C.S, Weil, U.C. Pozzani and J.A. Striegel (1962) Range finding toxicity data: List Vl. Industrial Hygiene Assn. J. 23: 95-107.

Substance Name	Heptanoic acid (data for homologue, octanoic acid) (mixed isomers)
CAS No.	124-07-2
Method/guideline	Oral LD50
Test Type	Oral LD50
GLP	No
Year	1962
Species/strain	Rat/Wistar
Sex	Male
# of animals per sex per dose	5
Vehicle	Not specified
Route of Administration	Oral
Remarks for Test Conditions	Chemicals administered undiluted (if possible) or diluted in water, corn oil or 1% TERGITOL via gastro-intubation.
Value LD50 or LC50 with confidence limits	LD50 = 1.41 (0.88-2.29) mL/kg or 1283 mg/kg
Number of deaths at each dose level	Not reported
Conclusion Remarks	Oral LD50 = 1.41 (0.88-2.29) mL/kg or 1283 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	No details given regarding doses and mortality.
References	Smyth Jr., H.F., C. P. Carpenter, C.S, Weil, U.C. Pozzani and J.A. Striegel (1962) Range finding toxicity data: List Vl. Industrial Hygiene Assn. J. 23: 95-107.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	LD50/calculated
Test Type	LD50
GLP	No
Year	1976
Species/strain	Rats/albino
Sex	Male and Female

# of animals per sex per dose	4
Vehicle	No vehicle used
Route of Administration	Oral
Value LD50 or LC50 with confidence limits	Oral LD50 = 8,370 (std. dev. +/- 1203 mg/kg)
Number of deaths at each dose level	1350 mg/kg, 0/4; 4556 mg/kg, 0/4; 6834 mg/kg, 1/4; 10,250 mg/kg, 3/4; 15,380 mg/kg, 4/4
Remarks for Results	Symptoms increasing in duration and severity with dose included hypoactivity, salivation, labored breathing, muscular weakness and prostration. Necropsy of dead animals revealed hemorrhaged lungs. At 2 highest doses, animals exhibited burns to GI tract.
Conclusion Remarks	Heptanoic acid was concluded to be practically nontoxic
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions
Remarks for Data Reliability	Although a small number of animals were used at each dose, results are consistent with other oral LD50 values.
References	Harrison W.A. (1976a) Acute Oral Toxicity Studies with heptanoic acid (SN1767). Industrial Biotest Laboratories, P.O. No. 045-858-76. Private Communication to FFHPVC. Unpublished report.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Dermal LD50
Test Type	Dermal LD50
GLP	No
Year	1974
Species/strain	Rabbit
Sex	Not reported
# of animals per sex per dose	10
Vehicle	Not reported
Route of Administration	Dermal
Remarks for Test Conditions	Animals given single dermal dose of 5 g/kg.
Value LD50 or LC50 with confidence limits	LD50 > 5000 mg/kg (no confidence limits reported)
Number of deaths at each dose level	No deaths reported
Remarks for Results	Symptoms reported include skin irritation: moderate redness (8/10), marked redness (2/10), moderate edema (7/10), and marked edema (3/10).

Conclusion Remarks	Dermal LD50=>5000 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Single dose to 10 animals.
References	Moreno O.M. (1974) Acute toxicity studies. Unpublished report to RIFM.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	Dermal LD50
Test Type	Dermal LD50
GLP	No
Year	1977
Species/strain	Rabbit
Sex	Not reported
# of animals per sex per dose	10
Vehicle	Not reported
Route of Administration	Dermal
Value LD50 or LC50 with confidence limits	LD50 > 5000 mg/kg
Number of deaths at each dose level	No deaths were described.
Remarks for Results	Clinical signs and observations included; 0/10 mortality, diarrhea in 1/10 on day 11, skin irritation; 10/10 reported to have severe redness, 10/10 reported to have moderate edema.
Conclusion Remarks	Dermal LD50 > 5000 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Single dose to 10 animals.
References	Moreno O.M. (1977) Acute toxicity studies. Unpublished report to RIFM.

Substance Name	Octanal (mixed isomers)
CAS No.	124-13-0
Method/guideline	Occluded 24 hr patch (Draize et al., 1944)
Test Type	Dermal LD50

GLP	No
Year	1962
Species/strain	Rabbit/albino New Zealand
Sex	Male
# of animals per sex per dose	4
Vehicle	Not reported
Route of Administration	Dermal
Remarks for Test Conditions	Fur was removed from entire trunk. The dose was applied beneath an impervious plastic. Animals immobilized during the 24-hour contact period after which the film was removed and the rabbits caged for the subsequent 14-day period.
Value LD50 or LC50 with confidence limits	LD50 = 6.35 mL/kg (4.70-8.59) or 5207 mg/kg
Number of deaths at each dose level	Not described
Remarks for Results	Based on mortalities during a 14-day observation period, the most probable LD50 value and its fiducial range are estimated by the method of Thompson (1947) using the tables of Weil (1952).
Conclusion Remarks	Dermal LD50 =6.35 mL/kg (4.70-8.59) or 5207 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	No detail regarding doses and mortality.
References	Smyth Jr., H.F., C. P. Carpenter, C.S, Weil, U.C. Pozzani and J.A. Striegel (1962) Range finding toxicity data: List Vl. Industrial Hygiene Assn. J. 23: 95-107.

Substance Name	Heptanoic acid (data for homologue, octanoic acid) (mixed isomers)
CAS No.	124-07-2
Method/guideline	Occluded 24 hr Patch (Draize et al., 1944)
Test Type	Dermal LD50
GLP	No
Year	1962
Species/strain	Rabbit/albino New Zealand
Sex	Male
# of animals per sex per dose	4
Vehicle	Not reported

Route of Administration	Dermal
Remarks for Test Conditions	Fur was removed from entire trunk. The dose was applied beneath an impervious plastic. Animals immobilized during the 24-hour contact period after which the film was removed and the rabbits caged for the subsequent 14-day period.
Value LD50 or LC50 with confidence limits	Dermal LD50 = 0.71 mL/kg or 647 mg/kg
Number of deaths at each dose level	Not described
Remarks for Results	No range was calculable because no dosage resulted in fractional mortality.
Conclusion Remarks	Dermal LD50 = 0.71 mL/kg or 647 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	No details given regarding doses and mortality.
References	Smyth Jr., H.F., C. P. Carpenter, C.S, Weil, U.C. Pozzani and J.A. Striegel (1962) Range finding toxicity data: List Vl. Industrial Hygiene Assn. J. 23: 95-107.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Dermal LD50
Test Type	Dermal LD50
GLP	No
Year	1971
Species/strain	Rabbit/albino
Sex	Not reported
# of animals per sex per dose	6
Vehicle	Not reported
Route of Administration	Dermal
Remarks for Test Conditions	Single dermal dose of 5 g/kg; applied on 3 rabbits with intact skin and 3 rabbits with abraded skin.
Value LD50 or LC50 with confidence limits	LD50 > 5000mg/kg
Number of deaths at each dose level	One death recorded on day 4.
Remarks for Results	Severe edema and burns at site of application.
Conclusion Remarks	Acute dermal LD50 = >5000 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.

References	Shelanski M.V. (1971) Acute toxicity studies in rats. Unpublished report to RIFM.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Dermal LD50
Test Type	LD50
GLP	No
Year	1976
Species/strain	Rabbits/albino
Sex	Male and Female
# of animals per sex per dose	4
Vehicle	No vehicle used
Route of Administration	Dermal
Value LD50 or LC50 with confidence limits	LD50 = >2000 mg/kg
Number of deaths at each dose level	2000 mg/kg, 1(M)/4
Remarks for Test Conditions	The material was applied undiluted to the abraided skin of 2 male and 2 female rabbits.
Remarks for Results	Body weights were reduced over the 14 day observation period. Skin changes at 24 hours included severe erythema, edema, and second and third degree burns. Necrosis was reported at skin sites at 14 days.
Conclusion Remarks	Heptanoic acid was concluded to be practically nontoxic
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions
Remarks for Data Reliability	Results are consistent with other oral LD50 values.
References	Harrison W.A. (1976b) Acute Dermal Toxicity Studies with heptanoic acid (SN1767). Industrial Biotest laboratories, P.O. No. 045-858-76. Private Communication to FFHPVC. Unpublished report.

Substance Name	Nonanal (data for nonanoic acid, 97%)
CAS No.	124-19-6
Method/guideline	Inhalation LC50
Test Type	Inhalation LC50
GLP	EPA GLP 40 CFR 792 (TSCA)

Year	1990
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
# of animals per sex per dose	10 (5M & 5F)
Vehicle	None
Route of Administration	Inhalation
Remarks for Test Conditions	Groups of Sprague-Dawley rats (5/sex) were exposed to aerosols containing a concentration of 0.046 or 3.8 mg/L of nonanoic acid for 4 hours. Exposure levels and particle size were measured 4 times. Animals were held for 14 day post-exposure.
Value LD50 or LC50 with confidence limits	LC50 between 0.46 and 3.8 mg/L (mean gravimetric exposure conc.) with a nominal concentration of 0.60 and 31 mg/L, respectively.
Number of deaths at each dose level	Eight (8) animals died at 3.8 mg/L. There were no mortalities at 0.46 mg/L.
Remarks for Results	Signs of irritation were noted during exposure and the first week post-exposure. Survivor's recovery within 14 days. Particle size distribution measurements showed average mass median diameter of 2.9 to 3.6 microns with 92% of the aerosol<10 microns.
Conclusion Remarks	The acute LC50 for nonanoic acid in male and female rats is > 0.46 mg/L but <3.8 mg/L.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Hoffman G. (1990) Acute inhalation toxicity study of nonanoic acid in the rat. Project No. 89-8216. Unpublished report to FFHPVC.

Substance Name	Heptanoic acid (98.5%)
CAS No.	111-14-8
Method/guideline	Inhalation LC50
Test Type	Inhalation LC50
GLP	EPA GLP 40 CFR 792 (TSCA)
Year	1990
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
# of animals per sex per dose	10 (5M & 5F)
Vehicle	None
Route of Administration	Inhalation

Remarks for Test Conditions	Groups of Sprague-Dawley rats (5/sex) were exposed to an aerosol containing a target concentration of 5.0 mg/L of heptanoic acid for 4 hours. Exposure levels and particle size were measured 4 times. Animals were held for 14 day post-exposure.
Value LD50 or LC50 with confidence limits	LC50 > 4.6 mg/L (mean gravimetric exposure conc.) with a nominal concentration of 28 mg/L.
Number of deaths at each dose level	Four animals died
Remarks for Results	Signs of irritation were noted during exposure and for several days post-exposure. Survivor's recovery within 14 days. Particle size distribution measurements showed average mass median diameter of 3.8 microns with 92% of the aerosol<10 microns.
Conclusion Remarks	LC50 > 4.6mg/L for male and female rats
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Hoffman G. (1990) Acute inhalation toxicity study of heptanoic acid in the rat. Project No. 89-8215. Unpublished report to FFHPVC.

Substance Name	Heptanal (90.8%)
CAS No.	111-71-7
Method/guideline	Inhalation LC50
Test Type	Inhalation LC50
GLP	EPA GLP 40 CFR 792 (TSCA)
Year	1989
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
# of animals per sex per dose	6 (3M & 3F)
Vehicle	None
Route of Administration	Inhalation
Remarks for Test Conditions	Groups of Sprague-Dawley rats (3/sex) were exposed to an atmosphere containing a target concentration of 5.0 mg/L of heptanal for 4 hours. Animals were observed at 15-minute intervals during the first hour exposure and daily post exposure.
Value LD50 or LC50 with confidence limits	LC50 > 4.7 mg/L (average exposure concentration)
Number of deaths at each dose level	No deaths recorded.
Remarks for Results	Nominal exposure concentration was 5.9 mg/L and average particle size was 0.80 mg/m^3.
Conclusion Remarks	LC50 > 4.7mg/L for male and female rats

Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Berardi, M.R. (1989) Acute inhalation toxicity study of heptanal in the rat. Project No. 88-8086. Unpublished report to FFHPVC.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	LD50/calculated per Miller and Tainter (1944).
Test Type	LD50
GLP	No
Year	1961
Species/strain	Mouse (strain not specified)
Sex	Male and Female
# of animals per sex per dose	6 groups of 10 mice per material
Vehicle	2% emulsion w cottonseed oil
Route of Administration	Injection (tail vein)
Value LD50 or LC50 with confidence limits	LD50 = 600 +/- 24 mg/kg
Number of deaths at each dose level	Not reported
Conclusion Remarks	Acute injected LD50 = 600 +/- 24 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Incomplete data on doses and strain.
References	Oro K. and A. Wretland (1961) Pharmacological effects of fatty acids, triolein and cottonseed oil. Acta Parmacol. Et Toxicol. 18:141-152.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	LD50/calculated per Miller and Tainter (1944).
Test Type	LD50
GLP	No
Year	1961
Species/strain	Mouse (strain not specified)
Sex	Male and Female

# of animals per sex per dose	6 groups of 10 mice per material
Vehicle	5% aqueous solution-cottonseed oil
Route of Administration	Injection (tail vein)
Value LD50 or LC50 with confidence limits	LD50 = 1200 +/- 56 mg/kg
Number of deaths at each dose level	Not reported
Conclusion Remarks	Acute injected LD50 = 1200 +/- 56 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Incomplete date (doses, strain)
References	Oro K. and A. Wretland (1961) Pharmacological effects of fatty acids, triolein and cottonseed oil. Acta Parmacol. Et Toxicol. 18:141-152.

4.2 In vitro Genotoxicity

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	Yes
Year	1992
Species/Strain	Salmonella typhimurium strains TA97, TA98, TA100, TA1535, TA1537
Metabolic Activation	Aroclor 1254-induced hamster or rat liver
Doses/Concentration	1, 3, 10, 33, 100, 166, 333, 1000, 1666, 3333 ug/plate
Remarks for Test Conditions	Preincubation procedure (Haworth et al 1983), with and without metabolic activation. Substance was considered mutagenic if it produced a reproducible, dose-related response over solvent control.
Results	Negative results in all strains with and without S9.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Heptanal not mutagenic

Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	Study performed by National Toxicology Program.
References	Zeiger, E., Anderson, B., Haworth, S., Lawlor, T., and Mortelmans, K. (1992). Salmonella mutagenicity tests: V. Results from the testing of 311 chemicals. Environ Molecul Mutagenesis 19(Suppl 21): 2-141.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	No
Year	1980
Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535, TA1537
Metabolic Activation	S9 mix from Aroclor 1254 or methylcholanthrene-induced rats
Doses/Concentration	3 umol/plate (402 ug/plate)
Statistical Methods	Average of two experiments
Remarks for Test Conditions	Test material was dissolved in ethanol.
Results	No increase in the incidence of reverse mutations with or without S9 activation.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Heptanal was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study lacked an adequate description of statistical methods.
References	Florin, I., L. Rutberg, M. Curvall and C.R. Enzell (1980) Screening of tobacco smoke constituents for mutagenicity using the Ames' Test. Toxicology, 18:219-232.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse mutation assay

System of Testing	Bacterial
GLP	No
Year	1980
Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535, TA1537
Metabolic Activation	S9 mix from Aroclor 1254 or methylcholanthrene-induced rats
Doses/Concentration	3 umol/plate (486 ug/plate)
Statistical Methods	Average of two experiments
Remarks for Test Conditions	Test material was dissolved in ethanol.
Results	There was no increase in the frequency of reverse mutations with or without S9 activation.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	The test material was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study lacked an adequate description of statistical methods.
References	Florin, I., L. Rutberg, M. Curvall and C.R. Enzell (1980). Screening of tobacco smoke constituents for mutagenicity using the Ames' Test. Toxicology 18:219-232.

Substance Name	Octanal
CAS No.	124-13-0
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	No
Year	1980
Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535, TA1537
Metabolic Activation	S9 mix from Aroclor 1254 or methylcholanthrene-induced rats
Doses/Concentration	3 umol/plate (444 ug/plate)
Statistical Methods	Average of two experiments
Remarks for Test Conditions	Test material was dissolved in ethanol.
Results	There was no increase in the frequency of reverse mutations with or without S9 activation.

Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	The test material was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study lacked an adequate description of statistical methods.
References	Florin, I., L. Rutberg, M. Curvall and C.R. Enzell (1980) Screening of tobacco smoke constituents for mutagenicity using the Ames' Test. Toxicology 18:219-232.

Substance Name	Nonanal (98%)
CAS No.	124-19-6
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Salmonella preincubation assay
System of Testing	Bacterial
GLP	Yes
Year	1986
Species/Strain	Salmonella typhimurium strains TA97, TA98, TA100, TA1535, TA1537
Metabolic Activation	S9 mix from Aroclor 1254-induced Sprague-Dawley rats
Doses/Concentration	0, 1, 3.5, 10, 35, 100, 355, 666 ug/plate
Statistical Methods	Not reported
Remarks for Test Conditions	Preincubation (48hrs), concurrent solvent and positive controls were tested with and without the metabolic activation systems, 7 dose levels and 3 plates per dose. All assays were repeated no less than 1 week after completion of the initial test.
Results	No increase in reverse mutations at any dose as compared to the solvent control.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Non mutagenic in this assay
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	Study performed by National Toxicology Program.
References	Mortelmans, K., S. Haworth, T. Lawlor, W. Speck, B. Tainer and E. Zeiger (1986). Salmonella mutagenicty tests: II. Results from the testing of 270 chemicals. Environ. Mutagen. 8(Suppl7): 1-119.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Ames (preincubation procedure) (Maron and Ames, 1983)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	No
Year	1985
Species/Strain	Salmonella typhimurium strains TA102, TA104
Doses/Concentration	Up to 1 mg/plate (1000 ug/plate)
Statistical Methods	Not reported
Remarks for Test Conditions	Test material was dissolved in either DMSO or water, preincubation with glutathione (end of preincubation period determined by time to decrease toxicity to long-chain alkenals)
Results	Maximum non-toxic dose = 0.4 umol/plate (65 ug/plate), no increase in reverse mutations.
Cytotoxic concentration	> 0.4 umol/plate
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was reported to show no evidence of mutagenicity in this assay.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study lacked an adequate description of statistical methods and doses.
References	Marnett, L.J., H.K. Hurd, M.C. Hollstein, D.E. Levin, H. Esterbauer and B.N. Ames (1985). Naturally occurring carbonyl compounds are mutagens in Salmonella tester strain TA104. Mutation Research 148:25-34.

Substance Name	Heptanal (data for a structurally related aldehyde, 5-heptenal, 2,6-dimethyl)
CAS No.	111-71-7
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	NG
Year	1983

Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535, TA1537, TA1538
Metabolic Activation	S9 liver fractions prepared from Aroclor-induced rats
Doses/Concentration	Five concentrations up to 3600 ug/plate
Statistical Methods	Kastenbaum and Bowman, 1970
Remarks for Test Conditions	Plates were incubated for 48 hours. DMSO used as a solvent for poorly soluble chemicals. Positive controls included 0.5 ug/plate of sodium azide for TA 1535 (430-760 revertants/plate) and TA 100 (400-700 revertants/plate) and 5ug/plate of benzo[a]pyrene for TA 100 (865-1210 revertants/plate), TA1537 235-350 revertants/plate), TA1538 (410-590 revertants/plate, and TA98 (660-1000 revertants/plate).
Results	No significant increased in reverse mutations.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Specific doses not reported and details of specific chemical not described. Data presented in tabular form.
References	Wild, D., M.-T. King, E. Gocke and K. Eckhardt (1983). Study of artificial flavouring substances for mutagenicity in the Salmonella /Microsome, BASC and micronucleus tests. Fd. Chem. Toxic. 21:707-719

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Ames assay (Ames et al., 1973; McCann et al., 1975)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	NG
Year	1989
Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535, TA1537, TA1538
Metabolic Activation	S9 fraction of Aroclor 1254-induced Sprague-Dawley rat liver
Doses/Concentration	Up to 150,000 ug/plate
Remarks for Test Conditions	Bacteria were culture in Oxford medium #2 for 12 hours. Assays were conducted by addition of 2.0 ml of test article to agar along with 0.1 ml of bacterial culture and either metabolic activation mix or an equivalent volume of phosphate buffer. The mixture was incubated for 48 hours and revertant colonies counted.

Results	No increase in reverse mutations, with or without S9 mix.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Heptanoic acid was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Heck, J.D., T.A. Vollmuth, M.A. Cifone, D.R. Jagannath, B. Myhr and R.D. Curren (1989). An evaluation of food flavoring ingredients in a genetic toxicity screening battery. The Toxicologist 9(1): 257.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	Ames assay (Ames et al., 1973; McCann et al., 1975)
Test Type	Reverse mutation assay
System of Testing	Bacterial
GLP	NG
Year	1989
Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535, TA1537, TA1538
Metabolic Activation	S9 fraction of Aroclor 1254-induced Sprague-Dawley rat liver
Doses/Concentration	Up to 50000 ug/plate
Remarks for Test Conditions	Bacteria were culture in Oxford medium #2 for 12 hours. Assays were conducted by addition of 2.0 ml of test article to agar along with 0.1 ml of bacterial culture and either metabolic activation mix or an equivalent volume of phosphate buffer. The mixture was incubated for 48 hours and revertant colonies counted.
Results	No increase in reverse mutations, with or without S9 mix.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Octanoic acid was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Heck, J.D., T.A. Vollmuth, M.A. Cifone, D.R. Jagannath, B. Myhr and R.D. Curren (1989). An evaluation of food flavoring ingredients in a genetic toxicity screening battery. The Toxicologist 9(1): 257.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse Mutation Assay
System of Testing	Bacterial
GLP	Yes
Year	1980
Species/Strain	Salmonella typhimurium TA1537, TA1538, TA98
Metabolic Activation	Aroclor 1254-induced hamster or rat liver
Doses/concentration levels	0.0001 to 0.01 ul/plate
Remarks for Test Conditions	A solution of the test article, positive controls or solvent control were mixed with the test organisms and applied to agar plates. The plates were then incubated at 37 °C for 48 hours. A positive mutagenesis concluded if it produced a reproducible, dose-related increase in reverse mutants is 2 to 3 times that for solvent control. Positive controls included 2-nitrofluorene for TA98 and TA1538 and 9-aminoacridine for TA1537.
Results	Negative results in all strains at all concentrations with and without S9.
Cytotoxic concentration	0.01 ul/plate
Genotoxic effects	None reported
Remarks for results	Tests using TA100 and TA1535 were discarded because of bacterial contamination.
Conclusion Remarks	Under these test conditions and according to the evaluation criteria, heptanal was not mutagenic in Salmonella typh. Stains TA 98, TA 1537, and TA1538 with or without metabolic activation.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Jagannath D.R. (1980) Mutagenic evaluation of C-191 in the Ames salmonella/microsome plate test. Project no. 20988. Unpublished report to FFHPVC.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse Mutation Assay

System of Testing	Bacterial
GLP	Yes
Year	1980
Species/Strain	Salmonella typhimurium TA1537, TA1538, TA98
Metabolic Activation	Aroclor 1254-induced hamster or rat liver
Doses/concentration levels	0.0001 to 0.01 ul/plate
Remarks for Test Conditions	A solution of the test article, positive controls or solvent control were mixed with the test organisms and applied to agar plates. The plates were then incubated at 37 C for 48 hours. A positive mutagenesis concluded, if it produced a reproducible, dose-related increase in reverse mutants is 2 to 3 times that for solvent control. Positive controls included 2-nitrofluorene for TA98 and TA1538 and 9-aminoacridine for TA1537.
Results	Negative results in all strains at all concentrations with and without S9.
Cytotoxic concentration	0.01 ul/plate for TA 1537/ TA1538; > 0.01 ul TA98
Genotoxic effects	None reported
Remarks for results	Tests using TA100 and TA1535 were discarded because of bacterial contamination.
Conclusion Remarks	Under these test conditions and according to the evaluation criteria, nonanal was not mutagenic in Salmonella typh. Stains TA 98, TA 1537, and TA1538 with or without metabolic activation.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Jagannath D.R. (1980) Mutagenic evaluation of C-192 in the Ames salmonella/microsome plate test. Project no. 20988. Unpublished report to FFHPVC.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse Mutation Assay
System of Testing	Bacterial
GLP	Yes
Year	1989
Species/Strain	Salmonella typhimurium TA100, TA1535, TA1537, TA1538, TA98
Metabolic Activation	Aroclor 1254-induced hamster or rat liver
Doses/concentration levels	Five concentrations from 667 to 10,000 ug/plate with S9 and from 100 to 5000 ug/plate without S9

Remarks for Test Conditions	A solution of the test article, positive controls or solvent (DMSO) control were mixed with the tester strain in molten agar at 45 C and applied to agar plates. The plates were then incubated at 37 C for 48 hours. A positive mutagenesis concluded, if the test article produced a reproducible, dose-related increase in mean number of reverse mutants at least 2 times that for solvent control. Positive controls included 2-aminoanthracene and 2-nitrofluorene for TA98 and 1538, 2-aminoanthracene and sodium azide for TA 100 and TA1535, 2-aminoanthracene and ICR-191 for TA1537.
Results	Negative results in all strains at all concentrations with and without S9.
Cytotoxic concentration	>10000 ug/plate +S9 and >5000 ug/plate -S9
Genotoxic effects	None reported
Conclusion Remarks	Under these test conditions and according to the evaluation criteria, there was no evidence that heptanoic acid was mutagenic in Salmonella typhimurium strains TA 98, TA 100, TA1535, TA 1537, and TA1538 with metabolic activation at concentrations up to 10000 ug/plate and without metabolic activation at concentrations up to 5000 ug/plate..
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	San R.H. and Schadly, M.B. (1989) Salmonella/microsome plate incorporation mutagenicity assay with heptanoic acid. Study no. T87768.501. Unpublished report to FFHPVC.

Substance Name	Nonanal (data for nonanoic acid)
CAS No.	124-19-6
Method/guideline	Ames assay (Ames et al., 1975)
Test Type	Reverse Mutation Assay
System of Testing	Bacterial
GLP	Yes
Year	1989
Species/Strain	Salmonella typhimurium TA100, TA1535, TA1537, TA1538, TA98
Metabolic Activation	Aroclor 1254-induced hamster or rat liver
Doses/concentration levels	Five concentrations from 667 to 10,000 ug/plate
Remarks for Test Conditions	A solution of the test article, positive controls or solvent (DMSO) control were mixed with the tester strain in molten agar at 45 C and applied to agar plates. The plates were then incubated at 37 C for 48 hours. A positive mutagenesis concluded, if the test article produced a reproducible, dose-related increase in mean number of reverse mutants at least 2 times that for solvent control. Positive controls included 2-aminoanthracene and 2-nitrofluorene for TA98 and 1538, 2-

	aminoanthracene and sodium azide for TA 100 and TA1535, 2-aminoanthracene and ICR-191 for TA1537.
Results	Negative results in all strains at all concentrations with and without S9.
Cytotoxic concentration	>10000 ug/plate
Genotoxic effects	None reported
Conclusion Remarks	Under these test conditions and according to the evaluation criteria, there was no evidence that nonanoic acid was mutagenic in Salmonella typh. strains TA 98, TA 100, TA1535, TA 1537, and TA1538 with and without metabolic activation at concentrations up to 10000 ug/plate.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	San R.H. and Kruel C. (1989) Salmonella/microsome plate incorporation mutagenicity assay with pelargonic acid. Study no. T87769.501. Unpublished report to FFHPVC.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Mouse lymphoma assay (Clive et al., 1979)
Test Type	Mammalian mutation assay
System of Testing	Mouse lymphoma cell
GLP	NG
Year	1989
Species/Strain	L5178Y mouse lymphoma cell
Metabolic Activation	Induced rat liver S9 and cofactors
Doses/Concentration	900 ug/ml with S9, 600 ug/ml without S9
Remarks for Test Conditions	Thymidine kinase competent heterozygote was exposed to the test article in the presence or absence of S9. After a 4-hour exposure, cells were washed, incubated (48hrs) to allow phenotypic expression, and colonies were counted after 10-14 days growth. Mutant frequency calculated using the ratio of mutant to viable colonies cloned without selective medium.
Results	Negative at 900 ug/mL with S9 and weakly positive at 600 ug/mL without S9.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Heptanoic acid was not mutagenic in the presence of metabolic activation and weakly mutagenic without metabolic activation.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Heck, J.D., T.A. Vollmuth, M.A. Cifone, D.R. Jagannath, B. Myhr and R.D. Curren (1989). An evaluation of food flavoring

ingredients in a genetic toxicity screening battery. The Toxicologist 9(1): 257.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	Mouse lymphoma assay (Clive et al., 1979)
Test Type	Mammalian Mutation Assay
System of Testing	Mouse lymphoma forward mutation assay
GLP	NG
Year	1981
Species/Strain	L5178Y mouse lymphoma cell
Metabolic Activation	Aroclor 1254 from Fisher N344 male rats
Doses/concentration levels	0.78 to 100 nl/ml without S9, 6.25 to 250 ng/ml with S9
Remarks for Test Conditions	Thymidine kinase competent heterozygote cells were exposed to the test article in the presence or absence of S9. After a 4-hour exposure, cells were washed, incubated (48-hrs) to allow phenotypic expression, and colonies were counted after 10 days growth. Mutant frequency calculated using the ratio of mutant to viable colonies cloned without selective medium.
Results	No evidence of mutagenicity concentrations up to 100 nl/ml without metabolic activation and 250 nl/ml with metabolic activation.
Cytotoxic concentration	125 nl/ml without S9, >250 nl/ml with S9
Genotoxic effects	None reported
Remarks for results	Without metabolic activation, moderate toxicity was observed at 0.78 nl/ml and high toxicity (8.8 to 5.8 % relative growth) was observed for concentrations from 50 to 100 nl/ml. With metabolic activation, weak toxicity (69.3% rel. growth) was observed at 6.25 nl/ml and moderate toxicity (22.8 % rel. growth) was observed for the 250 nl/ml concentration.
Conclusion Remarks	Concentrations up to 100 nl/ml without metabolic activation and 250 nl/ml with metabolic activation did not result in any evidence of mutagenicity in the mouse lymphoma forward mutation assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Myhr B. (1981) Mutagenic an evaluation of heptanal in the mouse lymphoma forward mutation assay. LBI Project No. 20989. Unpublished Report to FFHPVC.

Substance Name	Nonanal
CAS No.	124-19-6

Method/guideline	Mouse lymphoma assay (Clive et al., 1979)
Test Type	Mammalian Mutation Assay
System of Testing	Mouse lymphoma forward mutation assay
GLP	NG
Year	1981
Species/Strain	L5178Y mouse lymphoma cell
Metabolic Activation	Aroclor 1254 from Fisher N344 male rats
Doses/concentration levels	0.0977 to 25 nl/ml without S9, 0.0977 to 50 nl/ml with S9 (trial 1) and 6.25 to 120 nl/ml (trial 2)
Remarks for Test Conditions	Thymidine kinase competent heterozygote cells were exposed to the test article in the presence or absence of S9. After a 4-hour exposure, cells were washed, incubated (48hrs) to allow phenotypic expression, and colonies were counted after 10 days growth. Mutant frequency calculated using the ratio of mutant to viable colonies cloned without selective medium. Three repeat trials were performed without activation and two with activation.
Results	No evidence of mutagenicity at concentrations up to 25 nl/ml without metabolic activation. Weak evidence of mutagenicity with metabolic activation in trail 2 (1.9 fold increase compared to controls) at cytotoxic (24% rel. growth) concentration of 25 nl/ml and 2.2 fold increase in mutational frequency at cytotoxic levels (10-15% rel. growth) of 60 and 120 nl/ml.
Cytotoxic concentration	31.3 nl/ml without S9, >250 nl/ml with S9
Genotoxic effects	Slight increase (2.2 fold) at 60 &120 nl/ml.
Remarks for results	Without metabolic activation, there is no evidence of toxicity even at cytotoxic levels. With metabolic activation, weak mutagenic activity is associated with high cytotoxicity concentration.
Conclusion Remarks	Concentrations up to 25 nl/ml of nonanal without metabolic activation show no evidence of mutagenicity. Cytotoxic concentration of 60 and 120 nl/ml with activation show weak evidence of mutagenicity.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Myhr B. (1981). Mutagenic an evaluation nonanal in the mouse lymphoma forward mutation assay. LBI Project No. 20989. Unpublished Report to FFHPVC.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Sister chromatid exchange (SCE)
Test Type	Cytogenetic assay

System of Testing	Rat hepatocytes
GLP	NG
Year	1993
Species/Strain	Female Fischer 344 rat hepatocytes
Doses/Concentration	0, 0.1, 1.0, 10 or 100 uM in DMSO/plate (0, 16.2, 162, 1620, or 16,200 ug/plate)
Statistical Methods	Student's t test (dependent variables)
Remarks for Test Conditions	Aldehyde solutions in DMSO were added to culture medium containing freshly prepared F344 rat hepatocytes by a collagenase perfusion technique. Isolated hepatocytes were plated at a density of 20,000 cells/plate. After 3 hours incubation medium was removed and cultures were washed twice and 5ml of medium containing insulin (10-7M). Approximately 20 hours after the exchange an aqueous solution of nonanal in DMSO (<1%) was added to the cultures to yield a final concentration of 0.1, 1.0, 10, or 100 uM. The cultures were then incubated for 3 hours. The medium was washed twice and supplemented with EGF (40 ng/ml) and bromodeosoxyuridine (10 uM). 48 Hours later Colcemid (0.4 ug/ml) were added and incubated for 3 hours. For chromosomal aberrations and sister chromatid exchange analysis, the medium was replaced with 2ml collagenase (0.5 mg/ml) and the plates were incubated for an additional 10 minutes. Twenty (20) well-spread second division metaphases were scored individually, except for concentrations with a very low rate.
Results	Significant increase in SCE at 0.1 and 10 uM/plate ($p<0.05$), and at 1 and 100 uM/plate ($p<0.01$). No dose-response relationship. Data for induction of SCE (mean +/- std deviation); Control; 0.75+/-0.05; 0.1 uM, 0.95+/-0.07; 1.0 uM, 1.05+/-0.09; 10 uM, 1.13+/-0.09; 100 uM, 1.01+/-0.09.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was reported to result in cytogenetic damage in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls, statistics and concentrations tested were described in detail.
References	Eckl, P.M., A. Ortner and H. Esterbauer (1993). Genotoxic properties of 4-hydroxyalkenals and analogous aldehydes. Mutation Research 290:183-192.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Cytogenetic assay (Eckl et al., 1987; Michalopoulos et al., 1982)
Test Type	Chromosomal aberrations
System of Testing	Non bacterial
GLP	No
Year	1990
Species/Strain	Fischer 344 rat hepatocytes
Doses/Concentration	0, 0.1, 1.0, 10 or 100 uM/plate (0, 16.2, 162, 1620, or 16,200 ug/plate)
Statistical Methods	Student's t test (independent variables)
Remarks for Test Conditions	Aldehyde solutions (1-40 uM in 0.9% NaCl) were added to culture medium containing freshly prepared rat hepatocytes. After 3 hours incubation medium was removed and cultures were washed twice and 5ml of medium containing epidermal growth factor (40 ng/ml) and bromodeosoxyuridine (10 uM) were added. 48 hours later Colcemid (0.4 ug/ml) were added and incubated for 3 hours. For chromosomal aberrations at least 20 metaphases were scored. The number of chromosomal aberrations is given per diploid cell (42 chromosomes).
Results	At 100 uM, there was an increase (32-fold) in aberrations compared to controls. The increase was not statistically significant because of the high standard deviation in the assay. Therefore, there was no statistically significant increase in chromosomal aberrations in this assay. Control; 0.015+/-0.03; 0.1 uM, 0.31+/-0.2; 1.0 uM, 0.17+/-0.35; 10 uM, 0.19+/-0.32; 100 uM, 0.49+/-0.70
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls, statistics and concentrations tested were described in detail.
References	Esterbauer, H., P. Eckl and A. Ortner (1990) Possible mutagens derived from lipids and lipid precursors. Mutation Research, (238), 223-233.

Substance Name	Nonanal
CAS No.	124-19-6

Method/guideline	Cytogenetic assay (Eckl et al., 1987; Michalopoulos et al., 1982)
Test Type	Micronuclei
System of Testing	Rat hepatocytes
GLP	No
Year	1990
Species/Strain	Fischer 344 rat hepatocytes
Doses/Concentration	0, 0.1, 1.0, 10 or 100 uM/plate (0, 16.2, 162, 1620, or 16,200 ug/plate)
Statistical Methods	Student's t test (dependent variables)
Remarks for Test Conditions	Aldehyde solutions (1-40 uM in 0.9% NaCl) were added to culture medium containing freshly prepared rat hepatocytes. After 3 hours incubation medium was removed and cultures were washed twice and 5ml of medium containing epidermal growth factor (40 ng/ml) and bromodeosoxyuridine (10 uM) were added. 48 hours later Colcemid (0.4 ug/ml) were added and incubated for 3 hours. For micronuclei counts, cells were fixed and stained with DAPI. 1000 cells were scored to determine the % of mitotic cells and the % of cells with micronuclei.
Results	No significant increase in the frequency of micronuclei in micronucleated polychromatic erythrocytes. Data for % of cells with micronuclei (mean +/- std deviation); Control; 0.00; 0.1 uM, -1.01+/-6.19; 1.0 uM, 1.97+/-7.8; 10 uM, -3.77+/-7.5; 100 uM, 4.57+/-16.6.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not genotoxic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls, statistics and concentrations tested were described in detail.
References	Esterbauer, H., P. Eckl and A. Ortner (1990). Possible mutagens derived from lipids and lipid precursors. Mutat. Res. 238:223-233.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Cytogenetic assay (Eckl et al., 1987; Michalopoulos et al., 1982)
Test Type	Mitotic index
System of Testing	Rat hepatocytes
GLP	No

Year	1990
Species/Strain	Fischer 344 rat hepatocytes
Doses/Concentration	0, 0.1, 1.0, 10 or 100 uM/plate (0, 16.2, 162, 1620, or 16,200 ug/plate)
Statistical Methods	Student's t-test (for independent variables)
Remarks for Test Conditions	Aldehyde solutions (1-40 uM in 0.9% NaCl) were added to culture medium containing freshly prepared rat hepatocytes. After 3 hours incubation medium was removed and cultures were washed twice and 5ml of medium containing epidermal growth factor (40 ng/ml) and bromodeosoxyuridine (10 uM) were added. 48 hours later Colcemid (0.4 ug/ml) were added and incubated for 3 hours. For micronuclei counts, cells were fixed and stained with DAPI. 1000 Cells were scored to determine the % of mitotic cells and the % of cells with micronuclei.
Results	No significant increase in the frequency of mitotic index. Data for % of mitotic cells (mean +/- std deviation); Control; 0.41+/-0.16; 0.1 uM, 0.44+/-0.31; 1.0 uM, 0.41+/-0.22; 10 uM, 0.46+/-0.28; 100 uM, 0.52+/-0.37.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls, statistics and concentrations tested were described in detail.
References	Esterbauer, H., P. Eckl and A. Ortner (1990). Possible mutagens derived from lipids and lipid precursors. Mutation Research 238:223-233.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Cytogenetic assay
Test Type	Cytogenetic assay
System of Testing	Rat hepatocytes
GLP	NG
Year	1993
Species/Strain	Female Fischer 344 rat hepatocytes
Doses/Concentration	0, 0.1, 1.0, 10 or 100 uM in DMSO/plate (0, 16.2, 162, 1620, or 16,200 ug/plate)
Statistical Methods	Student's t test (dependent variables)

Remarks for Test Conditions	Aldehyde solutions in DMSO were added to culture medium containing freshly prepared F344 rat hepatocytes by a collagenase perfusion technique. Isolated hepatocytes were plated at a density of 20,000 cells/plate. After 3 hours incubation medium was removed and cultures were washed twice and 5ml of medium containing insulin (10-7M). Approximately 20 hours after the exchange an aqueous solution of nonanal in DMSO (<1%) was added to the cultures to yield a final concentration of 0.1, 1.0, 10, or 100 uM. The cultures were then incubated for 3 hours. The medium was washed twice and supplemented with EGF (40 ng/ml) and bromodeosoxyuridine (10 uM). 48 hours later Colcemid (0.4 ug/ml) was added and incubated for 3 hours. 1000 cells were analyzed under the fluorescence microscope.
Results	No significant increase in the frequency of micronuclei in micronucleated polychromatic erythrocytes. Data for increase in frequency of micronuclei (mean +/- std deviation); Control; 12.82+/-8.4; 0.1 uM, 10.64+/-7.3; 1.0 uM, 14.8+/- 10.6; 10 uM, 7.68+/-2.36; 100 uM, 16.0+/-18.9.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Non-mutagenic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls, statistics and concentrations tested were described in detail.
References	Eckl, P.M., A. Ortner and H. Esterbauer (1993). Genotoxic properties of 4-hydroxyalkenals and analogous aldehydes. Mutation Research 290:183-192.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Chromosomal aberration assay
Test Type	Cytogenetic assay
System of Testing	Rat hepatocytes
GLP	NG
Year	1993
Species/Strain	Female Fischer 344 rat hepatocytes
Doses/Concentration	0, 0.1, 1.0, 10 or 100 uM in DMSO/plate (0, 16.2, 162, 1620, or 16,200 ug/plate)
Statistical Methods	Student's t test (dependent variables)
Remarks for Test Conditions	Aldehyde solutions in DMSO were added to culture medium containing freshly prepared F344 rat hepatocytes by a collagenase perfusion technique. Isolated hepatocytes were

	plated at a density of 20,000 cells/plate. After 3 hours incubation medium was removed and cultures were washed twice and 5ml of medium containing insulin (10-7M). Approximately 20 hours after the exchange an aqueous solution of nonanal in DMSO (<1%) was added to the cultures to yield a final concentration of 0.1, 1.0, 10, or 100 uM. The cultures were then incubated for 3 hours. The medium was washed twice and supplemented with EGF (40 ng/ml) and bromodeosoxyuridine (10 uM). 48 Hours later Colcemid (0.4 ug/ml) were added and incubated for 3 hours. For chromosomal aberrations and sister chromatid exchange analysis, the medium was replaced with 2ml collagenase (0.5 mg/ml) and the plates were incubated for an additional 10 minutes. Twenty (20) well-spread second division metaphases were scored individually, except for concentrations with a very low rate. Data collected on results of six experiments at each concentration.
Results	No increase in the incidence of chromosomal aberrations. Data for induction of chromosomal aberrations (mean +/- std deviation); Control; 0.01+/-0.03; 0.1 uM, 0.31+/-0.28; 1.0 uM, 0.17+/-0.35; 10 uM, 0.19+/-0.32; 100 uM, 0.49+/-0.70.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not genotoxic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls, statistics and concentrations tested were described in detail.
References	Eckl, P.M., A. Ortner and H. Esterbauer (1993). Genotoxic properties of 4-hydroxyalkenals and analogous aldehydes. Mutation Research 290:183-192.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Unscheduled DNA synthesis (Williams, 1977)
Test Type	Unschedule DNA synthesis assay
System of Testing	Rat hepatocytes
GLP	NG
Year	1994
Species/Strain	Sprague-Dawley male albino rat hepatocytes
Doses/Concentration	0, 3, 10, 30, 100 mM
Statistical Methods	Student's t-test (two-tailed)
Remarks for Test Conditions	Cultures exposed for 20 hours to n-alkanals and 10 uCi/mL [methyl-3H]thymidine and were processed immediately after treatment for the autoradiographic evaluation of UDS.

	Substance was evaluated in 2 independent tests, nuclear grain counts of 200 cells. Positive and negative controls were n-dimethylnitrosoamine and solvent, respectively.
Results	No increase in unscheduled DNA synthesis.
Cytotoxic concentration	100 mM
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not genotoxic in this assay
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Martelli, A., R. Canonero, M. Cavanna, M. Ceradelli and U. Marinari (1994) Cytotoxic and genotoxic effects of five n-alkanals in primary cultures of rat and human hepatocytes. Mutation Research, 323:121-126.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	Unscheduled DNA synthesis (Williams, 1977)
Test Type	Unschedule DNA synthesis assay
System of Testing	Human hepatocytes
GLP	NG
Year	1994
Species/Strain	Human hepatocytes
Doses/Concentration	0, 3, 10, 30, 100 mM
Statistical Methods	Student's t-test (two-tailed)
Remarks for Test Conditions	Human hepatocyte suspensions were prepared from apparently healthy fragments of human liver discarded during the course of prescribed surgery (Strom et al., 1982). Cultures exposed 20 hours to n-alkanals and 10 uCi/mL [methyl-3H]thymidine and were processed immediately after treatment for the autoradiographic evaluation of UDS. Substance was evaluated in 2 independent tests, nuclear grain counts of 200 cells. Positive and negative controls were n-dimethylnitrosoamine and solvent, respectively.
Results	No increase in unscheduled DNA synthesis.
Cytotoxic concentration	100 mM
Genotoxic effects	None reported
Conclusion Remarks	Nonanal was not genotoxic in this assay.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions

References	Martelli, A., R. Canonero, M. Cavanna, M. Ceradelli and U. Marinari (1994). Cytotoxic and genotoxic effects of five n-alkanals in primary cultures of rat and human hepatocytes. Mutation Research 323:121-126.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Unscheduled DNA synthesis (Williams, 1977, 1980; Buttersworth et al., 1987)
Test Type	Unschedule DNA synthesis assay
System of Testing	Rat hepatocytes
GLP	Not reported
Year	1989
Species/Strain	Fischer or Sprague-Dawley rat hepatocytes
Doses/Concentration	1000 ug/ml
Remarks for Test Conditions	Cultures were incubated for 18-20 hrs with the test article. Unscheduled DNA synthesis measured by electronically counting nuclear grains in the nucleus and in 3 adjacent nuclear-sized cytoplasmic areas, for each dose level. Either 75 or 150 cells were analyzed. Net grains counts for the nucleus and cytoplasm were recorded. Positive UDS was indicated by an increase of at least 6 net grains per nucleus as compared to the solvent control. Negative control was DMSO and positive control was 2-acetylaminofluorene (AAF).
Results	No evidence of UDS at 1000 ug/mL.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Heptanoic acid was not genotoxic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The controls and other methodology were complete.
References	Heck, J.D., T.A. Vollmuth, M.A. Cifone, D.R. Jagannath, B. Myhr and R.D. Curren (1989). An evaluation of food flavoring ingredients in a genetic toxicity screening battery. The Toxicologist 9(1): 257.

Substance Name	Heptanoic acid (data for homologue, octanoic acid)
CAS No.	124-07-2
Method/guideline	Unscheduled DNA synthesis (Williams, 1977, 1980; Buttersworth *et al*., 1987)

Test Type	Unschedule DNA synthesis assay
System of Testing	Rat hepatocytes
GLP	NG
Year	1989
Species/Strain	Fischer or Sprague-Dawley rat hepatocytes
Remarks for Test Conditions	Cultures were incubated for 18-20 hours with the test article. Unscheduled DNA synthesis measured by electronically counting nuclear grains in the nucleus and in 3 adjacent nuclear-sized cytoplasmic areas, for each dose level. Either 75 or 150 cells were analyzed. Net grains counts for the nucleus and cytoplasm were recorded. Positive unscheduled DNA synthesis was indicated by an increase of at least 6 net grains per nucleus as compared to the solvent control. Negative control was DMSO and positive control was 2-acetylaminofluorene (AAF).
Results	No evidence of UDS at 300 ug/mL.
Cytotoxic concentration	Not reported
Genotoxic effects	None reported
Conclusion Remarks	Octanoic acid was not genotoxic in this assay.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
References	Heck, J.D., T.A. Vollmuth, M.A. Cifone, D.R. Jagannath, B. Myhr and R.D. Curren (1989). An evaluation of food flavoring ingredients in a genetic toxicity screening battery. The Toxicologist 9(1): 257.

4.3 In vivo Genotoxicity

Substance Name	Heptanal (data for structurally related aldehyde, 5-heptenal, 2,6-dimethyl)
CAS No.	111-71-7
Method/guideline	BASC test on Drosophila was performed as reported in Eckhardt, King, Gocke and Wild, 1980.
Test Type	BASC test (Wurgler, Sobels and Vogel, 1977)
GLP	NG
Year	1983
Species/Strain	Insect, Drosophila melanogaster
Sex	Male and Female
Route of Administration	Feed

Doses/Concentration	25 mM
Exposure Period	48 hrs
Remarks for Test Conditions	The test substance to be fed to the flies was prepared in 5% saccharose, with addition of 2% ethanol and 2% Tween 80. Ethyl nitrite was administered to Drosophila males in gaseous form. To do this, flies were kept for 3 days in 1-liter bottle containing small amount of medium, and ethyl nitrite was injected into the tightly closed bottles.
Genotoxic effects	None
NOEL (C)/ LOEL (C)	25 mM
Remarks for Results	No mutagenic activity was demonstrated under the test conditions. Data for number of sex-linked recessive lethal chromosome. Brood I 6/1847; Brood II, 6/1811; Brood III, 4/1966. Control: Brood I, 42/18188; Brood II, 34/17734; Brood III, 50/16980.
Conclusion Remarks	No mutagenic activity was demonstrated under the test conditions
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed Journal Food and Chemical Toxicology.
References	Wild, D., King, M. -T., Gocke, E. and Eckhardt, K. (1983). Study of Artificial Flavouring Substances for Mutagenicity in the Salmonella/Microsome, BASC and Micronucleus Tests. Food and Chemical Toxicology 21(6): 707-719.

Substance Name	Heptanal (data for structurally related aldehyde, 5-heptenal, 2,6-dimethyl)
CAS No.	111-71-7
Method/guideline	Micronucleus test. NMRI mice were treated once with the test material. The mice were killed and bone-marrow smear was prepared 30 hours after the treatment. The smears were stained according to the method of Schmid & the slides were scored.
Test Type	Micronucleus test
GLP	NG
Year	1983
Species/Strain	NMRI mice
Sex	Male and Female
Route of Administration	Not given
Doses/Concentration	0, 420, 980, 1540 mg/kg
Exposure Period	Single intraperitoneal injection
Remarks for Test Conditions	Test material injected into 4 mice. The vehicle was olive oil.

Effect on mitotic index or PCE/NCE ratio by dose level and sex	At 0 mg/kg, 1.7=mean MNPE/1000NPE; At 420mg/kg, 1.0=mean MNPE/1000 NPE; At 980 mg/kg 1.5=MNPE/1000 NPE; At 1540 mg/kg, 2.2= MNPE/1000 NPE NPE=Normal Polychromatic erythrocytes; MNPE=Micronucleated Polychromatic erythrocytes.
Genotoxic effects	None
NOEL (C)/ LOEL (C)	1540 mg/kg
Statistical Evaluation	Kastenbaum and Bowman, 1970.
Remarks for Results	No mutagenic activity was detected under the test conditions.
Conclusion Remarks	No mutagenic activity was detected under the test conditions.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study was published in a peer-reviewed Journal Food and Chemical Toxicology.
References	Wild, D., King, M.-T., Gocke, E. and Eckhardt, K. (1983) Study of Artificial Flavouring Substances for Mutagenicity in the Salmonella/Microsome, BASC and Micronucleus Tests. Food and Chemical Toxicology 21(6): 707-719.

4.4 Repeat Dose Toxicity

Substance Name	Heptanal (data for structurally related aldehyde, 2,6-dimethylhept-5-en-1-al)
CAS No.	111-71-7
Method/guideline	90-day feeding study
GLP	NG
Year	1983
Species/strain	Rat/Wistar, pathogen free
Sex	Male and Female
Route of Administration	Diet
Doses/concentration Levels	0, 9, 37, 150 mg 2,6-dimethylhept-5-en-1-al/kg bw/day
Exposure Period	90 days
Frequency of Treatment	Daily
Control Group	Yes
Post Exposure Observation Period	None
Remarks for Test Conditions	After a 4-day acclimatization period, rats were divided randomly into four groups of 15 animals of each sex and maintained on

	diets to provide daily intakes of 0 (control), 10, 40 and 60 mg/kg bw/day for 13-14 weeks. Rats were examined daily for mortality and clinical signs. Rats were weighed twice weekly and food consumption was measured daily. Water intake was recorded twice weekly. Blood was collected from the retro-orbitol plexus at week 6 and from the aorta of anesthetized rats at week 13/14. Hematology examined hemoglobin concentration, erythrocyte count, packed cell volume and leucocyte count. Serum clinical chemistry was performed on serum at weeks 6 and 13/14. Urine samples were collected during week 6 and during the last week of the study and examined for volume, pH, glucose, blood, bile, ketones and protein. At the end of the study, the rats were necropsied and histopathological examination of major tissues and organs (29) were performed.
NOAEL (NOEL)	37 mg/kg/bw/d
LOAEL (LOEL)	150 mg/kg/bw/d
Actual Dose Received by Dose Level and Sex	9, 36.6, 149.2 (m); 8.9, 36.5,153.1 (f) mg/kg bw/d
Toxic Response/effects by Dose Level	At 150 mg/kg/body weight; slight decrease in renal concentrating ability was reported at week 6 in males and at week 14 in females. Serum glucose levels of both sexes were elevated as compared to the controls at 150 mg/kg bw/d. There were no evidence of histopathology to any tissue or organ including the testes and ovaries.
Statistical Evaluation	Student's t-test (99 and 95%)
Conclusion Remarks	Administration of these doses produced no marked toxic effects in the rats, treatment of the rats had no effect on body weights, food or water intake. The higher hemoglobin concentrations in treated groups were not considered to be adverse findings. The cause of the increased serum glucose level at the highest dose is unknown.
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Data Reliabilities Remarks	Study was published in a peer-reviewed journal.
References	Gaunt, I.F., G. Wright, R. Cottrell and S. D. Gangolli (1983) Short-term toxicity of 2,6-dimethylhept-5-en-1-al in rats. Journal of Food and Chemical Toxicology, 21(5): 543-549.

Substance Name	Octanal (data for a mixture containing blend of aldehydes; C-8: Octanal (4 ppm), C-9: Nonanal (9 ppm), C-10 (2.2 ppm), C-11 (6 ppm), C-12 (6 ppm), C-12 (6 ppm) and methyl nonyl acetaldehyde (8 ppm)
CAS No.	124-13-0
Method/guideline	90-day feeding study
GLP	No
Year	1958
Species/strain	Rat

Sex	Male and Female
Route of Administration	Diet
Doses/concentration Levels	112 mg aliphatic aldehyde mixture/kg bw/d
Exposure Period	90 days
Frequency of Treatment	Daily
Control Group	Yes, basal diet only
Post Exposure Observation Period	None
Remarks for Test Conditions	Groups of 12 rats were maintained on diets containing 100 mg/kg bw of aldehyde mixture for 12 weeks. Controls were maintained on an unsupplemented diet. After 12 weeks, urine samples were examined for presence of sugar and albumin, and blood hemoglobin levels. At necropsy, liver and kidney weights were measured and the liver and kidneys were subjected to histopathological examination.
NOAEL (NOEL)	112 mg/kg bw/d
LOAEL (LOEL)	Not reported
Actual Dose Received by Dose Level and Sex	112 mg/kg body weight
Statistical Evaluation	Not reported
Remarks for Results	There was no effect on growth, food intake, or efficiency of food utilization. Based on hematological examination urine analysis, liver and kidney weights and histopathological examination of liver and kidney tissues, there was no evidence of toxicity associated with administration of the test substance.
Conclusion Remarks	The authors reported no adverse effects on growth, food intake, efficiency of food utilization or other physiological criteria (survival, body weight, behavior, appearance, urinalysis, blood hemoglobin, liver and kidney weights)
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Data Reliabilities Remarks	Study performed under contract to Food and Drug Administration. It was part of a screening program in which limited clinical chemistry, hematology, and histopathology was performed.
References	Trubeck Laboratories (1958) Toxicological examination of blend of aliphatic aldehydes in rats. Class III, Part 2. Unpublished report.

Substance Name	Heptanal (data for structurally related aldehyde, 5-heptenal, 2,6-dimethyl)
CAS No.	111-71-7
Method/guideline	29-day oral gavage study
GLP	Yes (CFR Pt 58, 1978)

Year	1990
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
Route of Administration	Gavage
Doses/concentration Levels	0, 300, 1500, and 3000 mg/kg bw/day
Exposure Period	29 days
Frequency of Treatment	Daily
Control Group	Yes (vehicle only)
Post Exposure Observation Period	None
Remarks for Test Conditions	Groups (10/sex/group) of rats, 44 days old were given the test substance by gavage in corn oil (10 ml/kg) daily for 29 days. Clinical signs were monitored twice weekly and body weights and food consumption were measured weekly. Baseline hematology and clinical chemistry were performed on 10 animals prior to initiation of the study. These animals were then discarded. At termination, all animals were fasted overnight. The animals were injected with ketamine and blood samples were drawn for clinical chemistry and hematology. At necropsy, organ weights were measured and tissues (26) were preserved in 10% formalin. All 26 tissues from controls and high-dose groups and the heart, liver, kidneys, and gross lesions from the low- and mid-dose group were embedded in paraffin, stained with hematoxylin and eosin, and examined microscopically.
NOAEL (NOEL)	300 mg/kg bw/day
LOAEL (LOEL)	1500 mg/kg bw/day
Toxic Response/effects by Dose Level	At 3000 mg/kg, 1 male and 3 females died during treatment. Other signs included languid behavior, prostration, ataxia and excess salivation. Clinical chemistry examination revealed increased alkaline phosphatase (males), increased total protein and albumin (both sexes). Significantly increased absolute and relative liver and kidney weights were accompanied by minimal centrilobular to diffuse hepatocellular hypertrophy, decreased periportal vaculization and increased hepatocellular cytoplasm density. In the kidney, male rats exhibited increased severity of hyaline droplets. Acanthosis was reported in the non-glandular stomach. 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 that could be related to administration of the test material.
Statistical Evaluation	Anova, then Dunnett's Comparison
Conclusion Remarks	Based on statistically significant changes in liver and kidney weights and histopathology of these organs 1500 mg/kg bw/day was considered the lowest observable adverse effect level (LOAEL) and 300 mg/kg bw/day was considered the no

	observable adverse effect level (NOAEL)
Data Qualities Reliabilities	Reliability Code 1. Reliable without restrictions.
Data Reliabilities Remarks	Study was conducted in compliance with Good Laboratory Practice Regulations, Title 21, U. S. Code of Federal Regulations Part 58
References	Terrill J. B. (1990a) 28-Day oral toxicity study in rats with 5-heptenal, 2,6-dimethyl. Lab. Project ID 642-482. Hazelton laboratories. Unpublished Report.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	27-day oral gavage study
GLP	Yes (CFR Pt 58, 1978)
Year	1990
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
Route of Administration	Gavage
Doses/concentration Levels	0, 875, 1750, and 3500 mg/kg bw/day
Exposure Period	27 days
Frequency of Treatment	Daily
Control Group	Yes (vehicle only)
Post Exposure Observation Period	None
Remarks for Test Conditions	Groups (10/sex/group) of rats 45 days of age were given the test substance by gavage in corn oil (10 ml/kg) daily for 27 days. Clinical signs were monitored twice weekly and body weights and food consumption were measured weekly. Baseline hematology and clinical chemistry were performed on 10 animals prior to initiation of the study. These animals were then discarded. At termination, all animals were fasted overnight. The animals were injected with ketamine and blood samples were drawn for clinical chemistry and hematology. At necropsy, organ weights were measured and tissues (26) were preserved in 10% formalin. All 26 tissues from controls and high-dose groups and the heart, liver, kidneys, and gross lesions from the low- and mid-dose groups were embedded in paraffin, stained with hematoxylin and eosin, and examined microscopically.
NOAEL (NOEL)	1750 mg/kg bw/day
LOAEL (LOEL)	3500 mg/kg bw/day

Toxic Response/effects by Dose Level	At 3500 mg/kg, 1 male and 5 females died during treatment. Five of the 6 deaths were considered related to gavage administration. Other signs included languid behavior, dyspnea, polypnea, tremors, wheezing, ataxia and excess salivation. Clinical chemistry and hematological examinations revealed no significant changes compared to those for the control group. A significant decrease in body weight and food consumption (males only) were recorded compared to those of the control group. Increased relative organ weight changes were not associated with a morphological change, but reflected lower terminal body weights. At necropsy, hyperkeratosis of the non-glandular stomach was reported in high-dose males and females. The rough and thickened mucosa of the non-glandular stomach noted at necropsy suggested a mild local irritation associated with gavage administration. At 875 and 1750 mg/kg bw/day dose levels, there were no significant findings that could be related to administration of the test material.
Statistical Evaluation	Yes. ANOVA, then Dunnett's Comparison
Conclusion Remarks	Based on decreased body weights and food consumption, gross lesions of the stomach, and microscopic lesions of the non-glandular region of the stomach, the 3500 mg/kg bw/day was considered the lowest observable adverse effect level (LOAEL). The dose level of 1750 mg/kg bw/day was considered the no observable adverse effect level (NOAEL).
Data Qualities Reliabilities	Reliability Code 1. Reliable without restrictions.
Data Reliabilities Remarks	Study was conducted in compliance with GLP Regulations, Title 21, U. S. Code of Federal Regulations Part 58
References	Terrill J. B. (1990b) 28-Day oral toxicity study in rats with heptanoic acid. Lab. Project ID 642-480. Hazelton Labs. Unpublished Report.

Substance Name	Heptanal (data for homologue, hexanal, 99%)
CAS No.	111-71-7
Method/guideline	28-day drinking water study
GLP	No
Year	1988
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
Route of Administration	Drinking water
Doses/concentration Levels	0.1, 0.9, 8.6, or 95.7 mg/kg/day/1.0, 10.0, 100.0, or 1000 mg/L
Exposure Period	28 days
Frequency of Treatment	Continuously
Control Group	0.05% Emuphor in water

Post Exposure Observation Period	None
Remarks for Test Conditions	Groups of SD rats (10/sex/group) were maintained on drinking water containing 1.0, 10.0, 100.0, or 1000 mg/L of hexanal for 4 weeks. Control groups received tap water and a vehicle control group received 0.5% Emuphor. Clinical observations were made daily and body weight, food and water consumption were made weekly. At necropsy brain, heart, liver, spleen and kidneys were weighed. At termination, hematological and clinical chemistry examinations were performed. Histopathology was performed on 26 tissues in controls and the highest exposure group.
NOAEL (NOEL)	95.7 mg/kg/day
Actual Dose Received by Dose Level and Sex	0.1, 0.9, 8.6, or 95.7 mg/kg/day
Toxic Response/effects by Dose Level	Based on measurement of body weight change, food and water consumption, hematological examination of the highest dose group, clinical chemistry examination, organ weights changes, and gross and histopathological examination, there were no significant differences between any treatment group and the control groups.
Statistical evaluations?	One-way analysis of variance.
Conclusion Remarks	There were no adverse effects related to the intake of up to 95.7 mg/kg/day of hexanal in drinking water.
Remarks for Results	Sporadic observations of dilated kidney pelvis (one animal at 10 mg/L and one at 100 mg/L) and hydronephrosis (one animal at 1000 mg/L) were not dose related and were no related to administration of the test material.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The study was performed at the Environmental and Occupational Toxicology Division, Environmental Health Directorate, Canada
References	Komsta E., Chu I., Secours V. E.,Valli V.E., Villeeneuve D. C. (1988) Results of a short-term toxicity study for three organic chemicals found in Niagara River drinking water. Bull. Environ. Contam. Toxicol, 41:515-522.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Mouse Skin Bioassay
GLP	Yes
Year	1985
Species/strain	Mouse C3H/HeJ
Sex	Male
Route of Administration	Dermal

Doses/concentration Levels	50 mg as a 75% solution in mineral oil
Exposure Period	80 weeks
Frequency of Treatment	Twice weekly
Control Group	Three control groups: Control group 1, no treatment; Control group 2, mineral oil; Positive control group 3, 0.05% benzo(a)pyrene in mineral oil.
Post Exposure Observation Period	None
Remarks for Test Conditions	Groups (50) of male mice were housed 5 per cage. Food and water were provided ad libitum. Mice were weighed weekly for the first month and thereafter every two weeks. Heptanoic acid (50 mg) in mineral oil, mineral oil (negative control), or 0.05% benzo(a)pyrene in mineral oil (positive control) was applied topically to the clipped interscapular region twice weekly. A second negative control group went untreated. Application continued for 80 weeks or until a neoplasm was clinically diagnosed as an "advanced tumor". During the study, animals were observed twice daily for signs of toxicity. A skin lesion that persisted for at least one week and grew to the size of approximately 1 mm, was classified as a papilloma. If the lesion grew and invaded surrounding tissue and became ulcerated and necrotic, it was diagnosed as an "advanced tumor". The skin was examined histologically for non-neoplastic and neoplastic lesions. Histological examination was performed on the organs of all animals at the conclusion of the study.
NOAEL (NOEL)	50 mg
Actual Dose Received by Dose Level and Sex	50 mg
Toxic Response/effects by Dose Level	Three of 50 mice treated with heptanoic acid developed benign skin tumors with a latent period of 65.7 weeks. Skin tumors were recorded for 45 of the 50 mice treated with 0.05% benzo(a)pyrene in mineral oil. One squamous cell carcinoma was reported in the untreated control group and no skin tumors were reported in the mineral oil group. The incidence of lesions in organs (e.g., hepatocarcinomas) of the negative control groups and test group were similar. Histologically the test group exhibited a slightly higher incidence of fibrosis and pigmentation of the skin.
Conclusion Remarks	Heptanoic acid (50 mg) administered to the skin of male mice twice weekly for 80 weeks did not show any evidence of carcinogenicity to the skin or other organs.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
References	Suskind R. (1985) Chronic mouse dermal toxicity study. Kettering Laboratory. Unpublished report.

Substance Name	Heptanal
CAS No.	111-71-7
Method/guideline	28-day dermal toxicity study

GLP	No
Year	1981
Species/strain	Rabbit/New Zealand White
Sex	Male and Female
Route of Administration	Dermal
Doses/concentration Levels	500 mg/kg/day
Exposure Period	Five days per week for two weeks
Frequency of Treatment	Daily
Control Group	Mineral
Post Exposure Observation Period	14 days
Remarks for Test Conditions	A single dose of 500 mg/kg of heptanal in mineral oil (25% solution) was applied to the freshly clipped lateral and dorsal areas of groups of rabbits (5/sex/group) daily for 5 days per week for 2 weeks. The skin of half the animals was abraded prior to the first, sixth, and eighth dose. A control group was treated with mineral oil only. Viability was recorded twice daily, observations for skin irritation were made daily, and body weights were measured weekly. After 2 weeks 6 animals (3 with abraided and 3 with intact skin) were necropsied with the remaining 4 animals sacrificed after an additional 2-week recovery period. Tissues from 29 organs were removed and preserved in 10% formalin.
NOAEL (NOEL)	<500 mg/kg/day
Actual Dose Received by Dose Level and Sex	500 mg/kg/day
Toxic Response/effects by Dose Level	No mortalities were observed at weeks 2 and 4. Most animals exhibited a weight loss after one or two weeks, but animals held for an additional two-week recovery period exhibited normal weight gain compared to controls. Most animals showed local dermal irritation reflected by slight to moderate erythema during the first week. Localized necrosis and exfoliation occurred in most animals during the second week. Microscopic evaluation revealed epidermal necrosis, epidermal hyperplasia, and hyperkeratosis at the application site. The skin application sites of animals held to week 4 appeared healed. The sites were re-epithelialized and continuous with normal follicular structure and population. No other microscopic alterations were reported for any other tissue that could be related to administration of the test material.
Statistical evaluations?	None
Conclusion Remarks	A single dose of 500 mg/kg of heptanal applied daily to the abraided and intact skin of rabbits 5 days per week for 2 weeks, resulted in site-specific irritation effects that were healed after a 2 week recovery period.

Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The only temporary effect, localized irritation involving necrosis, hyperkeratosis and exfoliation, healed in the 2-week post-treatment period.
References	Auletta C. (1981) A 28-day toxicity study in rabbits. Project No.6510-80. Unpublished report to FFHPVC.

Substance Name	Nonanal
CAS No.	124-19-6
Method/guideline	28-day dermal toxicity study
GLP	No
Year	1981
Species/strain	Rabbit/New Zealand White
Sex	Male and Female
Route of Administration	Dermal
Doses/concentration Levels	500 mg/kg/day
Exposure Period	Five days per week for two weeks
Frequency of Treatment	Daily
Control Group	Mineral
Post Exposure Observation Period	14 days
Remarks for Test Conditions	A single dose of 500 mg/kg of nonanal in mineral oil (25% solution) was applied to the freshly clipped lateral and dorsal areas of groups of rabbits (5/sex/group) daily for 5 days per week for 2 weeks. The skin of half the animals was abraded prior to the first, sixth, and eighth dose. A control group was treated with mineral oil only. Viability was recorded twice daily, observations for skin irritation were made daily, and body weights were measured weekly. After 2 weeks 6 animals (3 with abraided and 3 with intact skin) were necropsied with the remaining 4 animals sacrificed after an additional 2-week recovery period. Tissues from 29 organs were removed and preserved in 10% formalin.
NOAEL (NOEL)	<500 mg/kg/day
Actual Dose Received by Dose Level and Sex	500 mg/kg/day
Toxic Response/effects by Dose Level	No mortalities were observed at weeks 2 and 4. Several animals exhibited decreased food consumption during weeks 2 and 3. Most animals exhibited a weight loss after one or two weeks, but animals held for an additional two-week recovery period exhibited normal weight gain compared to controls. Most animals showed local dermal irritation reflected by slight to moderate erythema during the first week. Localized necrosis

	and exfoliation occurred in most animals during the second week. Microscopic evaluation revealed epidermal necrosis, epidermal hyperplasia, and hyperkeratosis at the application site. The skin application sites of animals held to week 4 appeared healed. The sites were re-epithelialized and continuous with normal follicular structure and population. No other microscopic alterations were reported for any other tissue that could be related to administration of the test material.
Statistical evaluations?	None
Conclusion Remarks	A single dose of 500 mg/kg of nonanal applied daily to the abraided and intact skin of rabbits 5 days per week for 2 weeks, resulted in site-specific irritation effects that were healed after a 2 week recovery period.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The only temporary effect, localized irritation involving necrosis, hyperkeratosis and exfoliation, healed in the 2-week post-treatment period.
References	Auletta C. (1981) A 28-day toxicity study in rabbits. Project No.6510-80. Unpublished report to FFHPVC.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	28-day dermal toxicity study
GLP	No
Year	1981
Species/strain	Rabbit/New Zealand White
Sex	Male and Female
Route of Administration	Dermal
Doses/concentration Levels	500 mg/kg/day
Exposure Period	Five days per week for two weeks
Frequency of Treatment	Daily
Control Group	Mineral
Post Exposure Observation Period	14 days
Remarks for Test Conditions	A single dose of 500 mg/kg of heptanoic acid in mineral oil (25% solution) was applied to the freshly clipped lateral and dorsal areas of groups of rabbits (5/sex/group) daily for 5 days per week for 2 weeks. The skin of half the animals was abraded prior to the first, sixth, and eighth dose. A control group was treated with mineral oil only. Viability was recorded twice daily, observations for skin irritation were made daily, and body weights were measured weekly. After 2 weeks 6 animals (3 with abraided and 3 with intact skin) were necropsied with the

	remaining 4 animals sacrificed after an additional 2-week recovery period. Tissues from 29 organs were removed and preserved in 10% formalin.
NOAEL (NOEL)	<500 mg/kg/day
Actual Dose Received by Dose Level and Sex	500 mg/kg/day
Toxic Response/effects by Dose Level	One mortality was recorded at day 11. Most animals exhibited a weight loss after two weeks, but animals held for an additional two-week recovery period exhibited normal weight gain compared to controls. All animals showed localized severe erythema, slight to severe edema, necrosis, desquamation and exfoliation by the second week of treatment. Some animals showed evidence of ocular irritation. Some animals showed decreased food consumption during the first 3 weeks of the study. All animals were free of signs of dermal and systemic toxicity at the end of the 2-week recovery period. Microscopic evaluation revealed epidermal necrosis, epidermal hyperplasia, and hyperkeratosis at the application site. The skin application sites of animals held to week 4 appeared healed. The sites were re-epithelialized and continuous with normal follicular structure and population. No other microscopic alterations were reported for any other tissue that could be related to administration of the test material.
Statistical evaluations?	None
Conclusion Remarks	A single dose of 500 mg/kg of heptanoic acid applied daily to the abraided and intact skin of rabbits 5 days per week for 2 weeks, resulted in site-specific irritation effects that were healed after a 2 week recovery period.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The only temporary effect, localized irritation involving necrosis, hyperkeratosis and exfoliation, healed in the 2-week post-treatment period.
References	Auletta C. (1981) A 28-day toxicity study in rabbits. Project No.6510-80. Unpublished report to FFHPVC.

Substance Name	Nonanal (data for metabolite, nonanoic acid)
CAS No.	124-19-6
Method/guideline	28-day dermal toxicity study
GLP	No
Year	1981
Species/strain	Rabbit/New Zealand White
Sex	Male and Female
Route of Administration	Dermal
Doses/concentration Levels	500 mg/kg/day

Exposure Period	Five days per week for two weeks
Frequency of Treatment	Daily
Control Group	Mineral
Post Exposure Observation Period	14 days
Remarks for Test Conditions	A single dose of 500 mg/kg of nonanoic acid in mineral oil (25% solution) was applied to the freshly clipped lateral and dorsal areas of groups of rabbits (5/sex/group) daily for 5 days per week for 2 weeks. The skin of half the animals was abraded prior to the first, sixth, and eighth dose. A control group was treated with mineral oil only. Viability was recorded twice daily, observations for skin irritation were made daily, and body weights were measured weekly. After 2 weeks 6 animals (3 with abraided and 3 with intact skin) were necropsied with the remaining 4 animals sacrificed after an additional 2-week recovery period. Tissues from 29 organs were removed and preserved in 10% formalin.
NOAEL (NOEL)	<500 mg/kg/day
Actual Dose Received by Dose Level and Sex	500 mg/kg/day
Toxic Response/effects by Dose Level	No mortalities were observed during the study. Most animals exhibited a weight loss after two weeks, but animals held for an additional two-week recovery period exhibited normal weight gain compared to controls. Most animals showed localized slight to severe erythema, slight to severe edema, necrosis, desquamation and exfoliation by the second week of treatment. Some animals showed evidence of ocular irritation. Some animals showed decreased food consumption during the weeks 2 and 3 of the study. All animals were free of signs of dermal and systemic toxicity at the end of the 2-week recovery period. Microscopic evaluation revealed epidermal necrosis, epidermal hyperplasia, and hyperkeratosis at the application site. The skin application sites of animals held to week 4 appeared healed. The sites were re-epithelialized and continuous with normal follicular structure and population. No other microscopic alterations were reported for any other tissue that could be related to administration of the test material.
Statistical evaluations?	None
Conclusion Remarks	A single dose of 500 mg/kg of nonanaoic acid applied daily to the abraided and intact skin of rabbits 5 days per week for 2 weeks, resulted in site-specific irritation effects that were healed after a 2 week recovery period.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	The only temporary effect, localized irritation involving necrosis, hyperkeratosis and exfoliation, healed in the 2-week post-treatment period.
References	Auletta C. (1981) A 28-day toxicity study in rabbits. Project No.6510-80. Unpublished report to FFHPVC.

4.5 Reproductive Toxicity

Substance Name	Heptanal (data for a structurally related aldehyde, 5-heptenal, 2,6-dimethyl)
CAS No.	111-71-7
Method/guideline	Virgin female Sprague-Dawley rats (10/group) were orally administered a vehicle or the test material at 3 dosages for one week prior to a 7-day cohabitation period through gestation, parturition and a 4-day postpartum period. Study duration was 39 days.
Test Type	Reproductive/Developmental study
GLP	GLP Regs. FDA (1987)
Year	1990
Species/Strain	Rat/Sprague-Dawley
Sex	Female/10/group
Route of Administration	Oral/gavage
Duration of Test	39 days
Doses/Concentration	0, 300, 1500 & 3000 mg/kg/day
Premating Exposure period for males	NG
Premating Exposure period for females	7 days
Frequency of Treatment	Daily
Control Group and Treatment	Corn Oil vehicle, 5 ml/kg/day
Remarks for Test Conditions	Mating, day 0 of gestation identified on basis of spermatozoa in vaginal smear. Viability was monitored twice daily during the study. Rats were observed daily for clinical signs approximately 30 minutes after gavage administration. Measurement of body weight was performed weekly. Food consumption measurement was also conducted weekly during the premating/premating period and then on days 0, 6, 14, 16, 21, and 25 of gestation and on days 1 and 4 of lactation/postparturition. Mating performance was evaluated daily during the cohabitation period. Dams were evaluated daily during gestation for duration of gestation, maternal behavior, litter size and pup viability. Dams that did not deliver litters were sacrificed on day 25 of presumed gestation and dams that did deliver litters were sacrificed on days 4 or 5 of lactation. All dams were examined for gross lesions and implantation sites. Ovaries from all dams and any observed gross lesions were preserved in neutral 10% formalin for possible evaluation. Vital signs at birth were determined for pups that were stillborn or died before the initial examination of the litter. Each litter was evaluated for viability a minimum of twice daily during the 4-day

	lactation period. Dead pups were removed and necropsied. Tissues with gross lesions were preserved for possible examination. Pups in each litter were counted and observed for nursing behavior and physical abnormalities daily. Pup body weights were measured on days 1 and 4 of postpurition.
NOAEL(NOEL)	300 mg/kg/d (maternal NOAEL)
LOAEL(LOEL)	1500 mg/kg/d (maternal)
Parental data and F1 as Appropriate	Clinical signs at 1500 and 3000 mg/kg in dams included decreased activity and excess salivation during the pre-gestation period and increased (P<0.01) salivation in the high dose group during gestation. Significant (P<0.05 to <0.01) decreases in body weight and absolute and relative food consumption were measured during the premating period. Eight rats of 10 in the high dose group were moribund or found dead on days 2, 3,and 4 of the premating period. Maternal body weights were decreased during gestation for the mid- and high-dose groups of dams. Decreased body weights and absolute and relative food consumption in the 300 mg/kg bw/day group occurred only during premating and were not considered adverse effects. One of the two surviving high-dose dames delivered a litter that died during the 4-day lactation period. Mating and fertility at the high dose were similar to controls. Measurements of mating success and fertility were similar for controls, low- and mid-dose groups.
Offspring Toxicity F1 and F2	Significant (P<0.05 to <0.01) decreases in pup viability occurred for middle and high dose groups as compared to controls. The mid-dose litters were significantly less (P<0.05) than control group litters. High-dose litters weighed remarkably less than controls. No changes in averages for duration of cohabitation or gestation, implantation sites or pup sex ratios were seen at any dose levels. No malformations or gross lesions in pups were attributable to the test material.
Statistical Evaluation	ANOVA followed by Dunnett's test
Remarks for Results	The decreased body weights and food consumption reported at 300 mg/kg bw/d during premating period were not considered adverse. Based on the significant decrease in (P<0.05) in pup weight at birth and pup viability in the mid-dose group, the NOAEL for the F1 offspring was reported to be >300 mg/kg bw/day but <1500 mg/kg bw/day.
Conclusion Remarks	Dose levels of 300 mg/kg bw/day of the test material (5-heptenal, 2,6-dimethyl) had no adverse effects on the reproductive performance of female Sprague-Dawley rats or the growth or development of their offspring.
Data Reliabilities Qualities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	Study met GLP Guidelines of U.S. Food and Drug Administration (1987) Good Laboratory Practice Guidelines; Final Rule. Fed. Reg. 9/4/87. Part VI, Vol. 52, No. 172. The study was published in a peer-reviewed journal, Teratology.
References	Vollmuth T.A., Bennett, M.B., Hoberman, A.M. and Christian, M.S. (1995) An Evaluation of Food Flavoring Ingredients Using an In Vivo Reproductive and Developmental Toxicity Screening Test. Teratology 41(5), 597.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Virgin female Sprague-Dawley rats (10/group) were orally administered a vehicle or the test material at 3 dosages for one week prior to a 7-day cohabitation period through gestation, parturition and a 4-day postpartum period. Study duration was 39 days
Test Type	Reproductive/Developmental Toxicity Study
GLP	GLP Regs. FDA (1987)
Year	1990
Species/Strain	Rat/Sprague-Dawley
Sex	Female/10/group
Route of Administration	Oral/gavage
Duration of Test	39 days
Doses/Concentration	0, 200, 1000 & 2000 mg/kg/day
Premating Exposure period for females	7 days
Frequency of Treatment	Daily
Control Group and Treatment	Corn Oil vehicle, 5 ml/kg/day
Remarks for Test Conditions	Mating, day 0 of gestation identified on basis of spermatozoa in vaginal smear. Viability was monitored twice daily during the study. Rats were observed daily for clinical signs approximately 30 minutes after gavage administration. Measurement of body weight was performed weekly. Food consumption measurement was also conducted weekly during the premating/premating period and then on days 0,6,14,16,21, and 25 of gestation and on days 1 and 4 of lactation/postparturition. Mating performance was evaluated daily during the cohabitation period. Dams were evaluated daily during gestation for duration of gestation, maternal behavior, litter size and pup viability. Dams that did not deliver litters were sacrificed on day 25 of presumed gestation and dams that did deliver litters were sacrificed on days 4 or 5 of lactation. All dams were examined for gross lesions and implantation sites. Ovaries from all dams and any observed gross lesions were preserved in neutral 10% formalin for possible evaluation. Vital signs at birth were determined for pups that were stillborn or died before the initial examination of the litter. Each litter was evaluated for viability a minimum of twice daily during the 4-day lactation period. Dead pups were removed and necropsied. Tissues with gross lesions were preserved for possible examination. Pups in each litter were counted and observed for nursing behavior and physical abnormalities daily. Pup body

	weights were measured on days 1 and 4 of postpurition.
NOAEL(NOEL)	<200 mg/kg/d (maternal NOAEL)
LOAEL(LOEL)	>1000 mg/kg/d (maternal)
Parental data and F1 as Appropriate	One and 3 deaths were reported in the 1000 and 2000 mg/kg bw/day dose groups, respectively. Clinical signs at 200 mg/kg bw/day in dams during premating and gestation included a significant increase in rales (P<0.01). This effect was not reported during the lactation period. In the 1000 and 2000 mg/kg bw/day dose group, significant increases in the incidence of rales (P<0.01), excess salivation (P<0.01) was reported during premating and gestation. Excess salivation continued during lactation in the high-dose group. Other significant (P<0.01) effects during gestation in the high-dose group included decreased activity, ungroomed coat and labored breathing. The 2000 mg/kg bw/day group showed reduced body weight gains during premating, and significantly (P<0.05 to <0.01) decreased average maternal body weights on days 10 and 16 of gestation. Average and relative food consumption was reduced in the high-dose group of dams throughout the study. The high dose also was associated with reduced mating and fertility that were related to mortality. The duration of cohabitation and fertility and gestation indices 200, 1000, or 2000 mg/kg bw/day were not different from comparable indices in thee control group.
Offspring Toxicity F1 and F2	The high-dose group exhibited reduced pup weights on day 4 postparturition. No biologically relevant or statistically significant differences in the number of implantations, duration of gestation, the percentage of dams delivering one or more live pups, and the pup viability index were observed. No malformations or gross lesions were observed in pups at any dose levels.
Statistical Evaluation	ANOVA followed by Dunnett's test
Remarks for Results	Based on the significant (P<0.01) increase of rales in the low-dose group of dams reported during premating and gestation period, the NOEAL for dams was <200 mg/kg bw/day. Based on reduced pup body weight on day 4 postpartum at the high dose, the NOAEL for the offspring was >1000 mg/kg bw/day and <2000 mg/kg bw/day.
Conclusion Remarks	Dose levels of 200 mg/kg bw/day of heptanoic acid had no significant adverse effects on the reproductive performance of female Sprague-Dawley rats or the growth or development of their offspring.
Data Reliabilities Qualities	Reliability code 1. Reliable without restrictions.
Remarks for Data Reliability	Study met GLP Guidelines of U.S. Food and Drug Administration (1987) Good Laboratory Practice Guidelines; Final Rule. Fed. Reg. 9/4/87. Part VI, Vol. 52, No. 172. The study was published in a peer-reviewed journal, Teratology.
References	Vollmuth T.A., Bennett, M.B., Hoberman, A.M. and Christian, M.S. (1995) An Evaluation of Food Flavoring Ingredients Using an In Vivo Reproductive and Developmental Toxicity Screening Test. Teratology 41(5): 597.

Substance Name	Heptanal
CAS No.	111-71-7
Test Type	Reproduction Study
GLP	No
Year	1941
Species/Strain	Rat/Wistar female, piebald
Sex	Female
Route of Administration	Oral (gavage)
Duration of Test	20 day
Doses/Concentration	0.50 ml/150-200 g female rat/day or 2050 mg/kg bw/day
Premating Exposure period for females	None reported
Frequency of Treatment	Daily
Control Group and Treatment	No control group
Remarks for Test Conditions	Several young female rats were mated with one male and the mating success was monitored by daily vaginal smears. Ten females were used in the study. Female rats were maintained on Purina Dog Chow and water ad libitum. Body weights were measured daily and the difference in weight between the weight on the day of insemination and immediately after parturition were also recorded. There was no reported of resorptions in any of the 10 female rats.
NOAEL(NOEL)	2050 mg/kg bw/day
Statistical Evaluation	None
Conclusion Remarks	Oral administration of 2050 mg/kg bw/day of heptanal resulted in no evidence of reproductive toxicity in female Wistar rats.
Data Reliabilities Qualities	Reliability code 3. Not reliable. Study contained measurement of limited number of parameters measuring reproduction.
Remarks for Data Reliability	Oral study was a preliminary study in Wistar rats. The results of the study were used to design a second study using the intraperitoneal route of administration. In the second study heptanal did not impair the reproductive system of rats.
References	Carruthers C. and Stowall R.E. (1941) Influence of heptaldehyde on the pregnancy in rats. Cancer Research, 1(9):724-728.

4.6 Developmental/Teratogenicity Toxicity

Substance Name	Octanal (data for a metabolite, octanoic acid
CAS No.	124-13-0
Method/guideline	Chernoff/Kalock assay
Test Type	Developmental toxicity
GLP	NG
Year	1994
Species/strain	Sprague-Dawley rat
Sex	Female
Route of Administration	Gavage
Duration of Test	28 days
Doses/concentration Levels	0, 1125, 1500 mg/kg/day
Exposure Period	10 days
Frequency of Treatment	Once daily (days 6-15 of gestation)
Control Group and Treatment	Controls used but were not defined.
Remarks for Test Conditions	High dose level expected to produce moderate maternal toxicity and the low dose was 75% of the high dose
LOAEL (LOEL) Maternal Toxicity	1125 mg/kg bw/d
NOAEL (NOEL) Developmental Toxicity	1125 mg/kg bw/d
Maternal Data with Dose Level	No effect on # of implants, but decreased body weight in dams at both dose levels.
Fetal Data with Dose Level	Significant decrease ($p<0.05$) in the number of live pups at the high dose only; no effect on perinatal loss (%) or pup weight at either dose.
Statistical Evaluation	Yes
Conclusion Remarks	Octanoic acid induced a significant decrease in the number of live pups in Sprague-Dawley rats but only at a dose, which causes maternal toxicity.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions. Study on development toxicity potential of a variety of organic acids. No visceral or skeletal examinations were performed.
Remarks for Data Reliability	Adequate number of animals, statistics, concentrations tested; but a limited discussion of data.
References	Narotsky, M.G., E.Z. Francis and R.J. Kavlock (1994) Developmental toxicity and structure-activity relationships of aliphatic acids including dose-response assessment of valproic

acid in mice and rats. Fundamental and Applied Toxicology 22:251-265.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Embryo/fetal and teratogenesis
Test Type	Embryo-fetotoxicity
GLP	NG
Year	1983
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
Route of Administration	Gavage
Duration of Test	20 days
Doses/concentration Levels	1000 mg/kg bw/day
Exposure Period	9 days (days 6-15 of gestation)
Frequency of Treatment	One daily (day 6-15)
Control Group and Treatment	Vehicle (Corn oil) only
Remarks for Test Conditions	Groups of male (1) and female (2) rats were bred until mating was confirmed. Following mating, a group of 22 female rats were given 1000 mg/kg of heptanoic acid daily for days 6 to 15 of pregnancy. Body weights and food consumption were measured regularly during gestation. On day 20 of gestation, females were sacrificed and the number of corpora lutea/ovary, implantation sites, early and late resorptions, and live and dead fetuses were recorded. One third of the fetuses received visceral examinations and two-thirds were subjected to skeletal examination. Dam uterine weights were measured and tissues from ovaries and uterus were preserved for microscopic examination. All data was subjected to ANOVA analysis (Dunnett's T-test)
NOAEL (NOEL) maternal toxicity	1000 mg/kg bw/day
NOAEL (NOEL) developmental toxicity	1000 mg/kg bw/day
Maternal data with dose level	Based on lack of mortality and clinical observations, no significant difference between body weight changes and food and water consumption for test and control animals, and the lack of any gross pathology, it was concluded that there was no maternal toxicity observed in this study.
Fetal Data with Dose Level	Based on mean ovarian, uterine, litter size, pregnancy rates, corpora lutea, implantation sites and efficiency, fetal viability, fetal size and sex, uterine weights, gross pathology, and

	visceral and skeletal examinations, there was no significant difference between the test and control group.
Statistical Evaluation	ANOVA (Dunnett's T-test)
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Conclusion remarks	There was no evidence of embryo toxicity, fetal toxicity, or teratogenesis when pregnant female rats were given 1000 mg/kg bw/day of heptanoic acid on days 6-15 of pregnancy.
References	Serota D.G. (1983) Evaluation of the embryo/fetal toxicity and teratogenic effects of a series of ten compounds in pregnant Sprague-Dawley rats. Project No 299-534. Unpublished Report to FFHPVC.

Substance Name	Nonanal (data for a metabolite, nonanoic acid)
CAS No.	124-19-6
Method/guideline	Embryo/fetal and teratogenesis
Test Type	Embryo-fetotoxicity
GLP	NG
Year	1983
Species/strain	Rat/Sprague-Dawley
Sex	Male and Female
Route of Administration	Gavage
Duration of Test	20 days
Doses/concentration Levels	1500 mg/kg bw/day
Exposure Period	9 days (days 6-15 of gestation)
Frequency of Treatment	One daily (day 6-15)
Control Group and Treatment	Vehicle (Corn oil) only
Remarks for Test Conditions	Groups of male (1) and female (2) rats were bred until mating was confirmed. Following mating, a group of 22 female rats were given 1000 mg/kg of nonanoic acid daily for days 6 to 15 of pregnancy. Body weights and food consumption were measured regularly during gestation. On day 20 of gestation, females were sacrificed and the number of corpora lutea/ovary, implantation sites, early and late resorptions, and live and dead fetuses were recorded. One third of the fetuses received visceral examinations and two-thirds were subjected to skeletal examination. Dam uterine weights were measured and tissues from ovaries and uterus were preserved for microscopic examination. All data was subjected to ANOVA analysis (Dunnett's T-test).
NOAEL (NOEL) maternal toxicity	1500 mg/kg bw/day

NOAEL (NOEL) developmental toxicity	1500 mg/kg bw/day
Maternal data with dose level	Based on lack of mortality and clinical observations, no significant difference between body weight changes and food and water consumption for test and control animals, and the lack of any gross pathology, it was concluded that there was no maternal toxicity observed in this study.
Fetal Data with Dose Level	Based on mean ovarian, uterine, litter size, pregnancy rates, corpora lutea, implantation sites and efficiency, fetal viability, fetal size and sex, uterine weights, gross pathology, and visceral and skeletal examinations there were no significant difference between the test and control group.
Statistical Evaluation	ANOVA (Dunnett's T-test)
Data Qualities Reliabilities	Reliability code 1. Reliable without restrictions.
Conclusion remarks	There was no evidence of embryo toxicity, fetal toxicity, or teratogenesis when pregnant female rats were given 1500 mg/kg bw/day of nonanoic acid on days 6-15 of pregnancy.
References	Serota D.G. (1983) Evaluation of the embryo/fetal toxicity and teratogenic effects of a series of ten compounds in pregnant Sprague-Dawley rats. Project No 299-534. Unpublished report to FFHPVC.

Substance Name	Heptanoic acid (data on homologue octanoic acid)
CAS No.	111-14-8
Test Type	Developmental Toxicity
GLP	NG
Year	1994
Species/strain	Sprague-Dawley rat
Sex	Female
Route of Administration	Oral (gavage)
Duration of Test	20 day of gestation
Doses/concentration Levels	18.75 mmol/kg (2700 mg/kg)
Exposure Period	One day
Frequency of Treatment	Single dose on day 20 of gestation
Control Group and Treatment	Controls received no test substance, not specified
Remarks for Test Conditions	All agents were administered undiluted by oral gavage on the morning of day 12 of rat gestation (day 0 = morning of finding vaginal plug). On day 20 of gestation, rats were killed by chloroform overdose, and survivability, # of implantation sites, and mean fetal weight were recorded.
NOAEL (NOEL) maternal toxicity	18.75 mmol/kg (2700 mg/kg)

Maternal data with dose level	Maternal toxicity considered severe at this dose level.
Fetal Data with Dose Level	Octanoic acid devoid of embryotoxic effects except for a slight reduction of fetal weight may be attributable to the severe maternal toxicity observed at the 2700 mg/kg dose.
Statistical Evaluation	None described
Data Qualities Reliabilities	Reliability code 3. Not reliable. Study was experimental in nature. Contained a limited number of measurements on development.
Remarks for Data Reliability	Lacking full description of controls and statistics.
Conclusion remarks	Octanoic acid was not embryotoxic in this assay.
References	Scott, Jr., W.J., M.D. Collins and H. Nau (1994) Pharmacokinetic determinants of embryotoxicity in rats associated with organic acids. Env. Health Perspectives, 102 (Suppl. 11) 97-101.

Substance Name	Octanal (data for metabolite of octanoic acid)
CAS No.	124-13-0
Method/guideline	Teratogenesis
Test Type	Developmental toxicity
GLP	NG
Year	1986
Species/strain	NMRI mice
Sex	Female
Route of Administration	Subcutaneous injection
Duration of Test	10 days
Doses/concentration Levels	0, 600 mg/kg body weight
Exposure Period	Single injection on day 8 of gestation
Frequency of Treatment	One
Control Group and Treatment	Control given water vehicle sc only.
Remarks for Test Conditions	Groups of 15 mice were treated on day 8. Examinations were performed on day 18 of gestation. Implantation sites were counted and each live fetus was individually weighed and inspected for the presence of neural tube defects.
Fetal Data with Dose Level	15% embryolethality (7% in controls); No effect on fetal weigh or on percentage of exencephaly in live fetuses.
Statistical Evaluation	Yes
Data Qualities Reliabilities	Reliability code 3. Not reliable. Experimental study in which a single dose was administered on day 8 of gestation. Fetal

	examination was limited to analysis of neural tube defects.
Remarks for Data Reliability	The study included an adequate number of animals, statistics, and concentrations tested, but a limited description of data. Published in a peer-reviewed journal.
References	Nau, H. and W. Loscher (1986) Pharmacologic evaluation of various metabolites and analogs of valproic acid: Teratogenic potencies in mice. Fund. Appl. Toxicol. 6:669-676.

Substance Name	Heptanoic acid
CAS No.	111-14-8
Method/guideline	Teratogenesis
Test Type	Frog embryo teratogenesis assay
GLP	NG
Year	1996
Species/strain	Xenopus embryos
Sex	Not reported
Route of Administration	In solution
Duration of Test	96 hrs
Doses/concentration Levels	8 concentrations (not specified) and 1 control
Exposure Period	96 hrs
Frequency of Treatment	Single exposure
Control Group and Treatment	Controls used but were not defined.
Remarks for Test Conditions	Embryos were collected following hormone-induced breed. Each group of 25 embryos was exposed to one of 8 concentrations of acid and a control, each acid was tested three times and data were pooled to calculate 96 hrs LC50 (lethality) and 96 hrs EC50 (malformation) and development hazard index (DHI).
Fetal Data with Dose Level	LC50 = 319.6 (313-324) mg/l; EC50 = 51.3 (48-55) mg/l; DHI = 6.2
Statistical Evaluation	Yes
Conclusion Remarks	Developmental hazard index was found to be greater than 5 indicating a moderate hazard according to the authors.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Study was published in a peer-reviewed journal.
References	Dawson, D.A., W. Schultz and R.S. Hunter (1996) Developmental toxicity of carboxylic acids to Xenopus embryos: A quantitative structure-activity relationship and computer-automated structure evaluation. Teratogenesis, Carcinogenesis

and Mutagenesis 16:109-124.

Substance Name	Heptanoic acid (data for homologue octanoic acid)
CAS No.	124-07-2
Method/guideline	Teratogenesis
Test Type	Frog embryo teratogenesis assay
GLP	NG
Year	1996
Species/strain	Xenopus embryos
Sex	Not reported
Route of Administration	In solution
Duration of Test	96 hrs
Doses/concentration Levels	8 concentrations (not specified) and 1 control
Exposure Period	96 hrs
Frequency of Treatment	Single exposure
Control Group and Treatment	Controls used but were not defined.
Remarks for Test Conditions	Embryos were collected following hormone-induced breed, each group of 25 embryo was exposed to one of 8 concentrations of acid and a control, each acid was tested three times and data were pooled to calculate 96h LC50 (lethality) and 96h EC50 (malformation) and development hazard index (DHI).
Fetal Data with Dose Level	LC50 = 127.1 (119-136) mg/l; EC50 = 28.1 (26-30) mg/l; DHI = 4.5
Statistical Evaluation	Yes
Conclusion Remarks	Developmental hazard index was found to be less than 5 indicating a low hazard according to the authors.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Study was published in a peer-reviewed journal.
References	Dawson D.A., W. Schultz and R.S. Hunter (1996) Developmental toxicity of carboxylic acids to xenopus embryos: a quantitative structure-activity relationship and computer-automated structure evaluation. Teratogenesis, Carcinogenesis and Mutagenesis 16:109-124.

Substance Name	Nonanal (data for metabolite of nonanal, nonanoic acid)
CAS No.	124-19-6
Method/guideline	Teratogenesis
Test Type	Frog embryo teratogenesis assay
GLP	NG
Year	1996
Species/strain	Xenopus embryos
Sex	Not reported
Route of Administration	In solution
Duration of Test	96 hrs
Doses/concentration Levels	8 concentrations (not specified) and 1 control
Exposure Period	96 hrs
Frequency of Treatment	Single exposure
Control Group and Treatment	Controls used but were not defined.
Remarks for Test Conditions	Embryos were collected following hormone-induced breed, each group of 25 embryo exposed to one of 8 concentrations of acid and a control, each acid was tested three times and data were pooled to calculate 96 hrs LC50 (lethality) and 96 hrs EC50 (malformation) and development hazard index (DHI).
Fetal Data with Dose Level	LC50 = 32.7 (29-36) mg/l; EC50 = 6.5 (6-7) mg/l; DHI = 5.0
Statistical Evaluation	Yes
Conclusion Remarks	DHI was found to be 5 indicating a low to moderate hazard according to the authors
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Study was published in a peer-reviewed journal.
References	Dawson D.A., W. Schultz and R.S. Hunter (1996) Developmental toxicity of carboxylic acids to xenopus embryos: a quantitative structure-activity relationship and computer-automated structure evaluation. Teratogenesis, Carcinogenesis and Mutagenesis 16:109-124.