AR 201-12876

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Gailen A. Hart
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December 21, 2000

Charles M. Auer
Director, Chemical Control Division
Office of Pollution Prevention and Toxics
US Environmental Protection Agency
401 M Street, S.W., MC 7405
Washington, DC 20460

Re: HPV Test Plan and Robust Summaries for C_6-C_{13} Alkyl Esters Category

Dear Mr. Auer:

Enclosed is the test plan for ExxonMobil Chemical Company's Alkyl Esters Category under the HPV Chemical Challenge Program. We are submitting robust summaries for existing data for the SIDS endpoints for substances included in this category. The test plan and robust summaries are also available electronically on the attached diskette.

If you have any questions, please contact me at 281-870-6309.

Regards,

Gailen A. Hart

MR-42661

AR 201-12939A

HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For The

ALKYL ACETATE C6 - Cl3 CATEGORY

Prepared by:

ExxonMobil Chemical Company

December 25, 2000

EXECUTIVE SUMMARY

Under EPA's High Production Volume (HPV) Challenge Program ExxonMobil Chemical Company has committed to voluntarily compile a Screening Information Data Set (SIDS) on a category of chemicals defined as Alkyl Acetates C6 - C13. This category is supported by the basic screening data needed for an initial assessment of the physicochemical properties, environmental fate, and human and environmental effects of chemicals as defined by the Organization for Economic Cooperation and Development (OECD). The information used to complete the HPV SIDS endpoints comes from existing data.

ExxonMobil Chemical Company believes a category of Alkyl Acetates C6 - Cl3 is scientifically justifiable because their physicochemical and toxicological properties are very similar and follow a regular pattern as a result of the synthesis process. The structural similarities create a predictable pattern in the following parameters: physicochemical properties, environmental fate and environmental effects, and/or human health effects. The similarities are based on the following: a common structure (CH_3COOR), an incremental and constant change across the category where R is a branched alkyl group having carbon numbers C6, C7, C8, C9, C10, or Cl3 as the main constituent, a common functional ester group, and a likelihood of common precursors and breakdown products which result in structurally similar chemicals (e.g., acetic acid and intermediate-chain aliphatic alcohols).

The test data compiled for the category anchor studies proves adequate to support a screening-level hazard assessment for the category and its members (CAS numbers, 88230-35-7, 90438-79-2, 108419-32-5, 108419-33-6, 108419-34-7, and 108419-35-8). One can assess the untested endpoints by extrapolation between and among the category members.

The use of an Alkyl Acetate C6 - Cl3 category will: First, inform the public earlier about any hazards of Alkyl Acetates C6 - Cl 3. Second, the matrix of completed anchor study testing demonstrates the safety of the category without end-point tests for each chemical. Third, this reduction in testing resulted in fewer animals used to test this category of chemicals as opposed to doing each test on individual Alkyl Acetates C6 - c13.

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TEST PLAN FOR ALKYL ACETATES C6 - Cl3

I. INTRODUCTION

Under EPA's High Production Volume (HPV) Challenge Program ExxonMobil Chemical Company has committed to voluntarily compile a Screening Information Data Set (SIDS) on a category of chemicals defined as Alkyl Acetates C6 - C13. This category is supported by the basic screening data needed for an initial assessment of the physicochemical properties, environmental fate, and human and environmental effects of chemicals as defined by the Organization for Economic Cooperation and Development (OECD). The information used to complete the SIDS comes from existing data and fulfills an ExxonMobil obligation to the HPV Challenge Program.

ExxonMobil Chemical Company believes a category of Alkyl Acetates C6 - Cl3 is scientifically justifiable because their physicochemical and toxicological properties are very similar and follow a regular pattern as a result of the synthesis process. The structural similarities create a predictable pattern in the following parameters: physicochemical properties, environmental fate and environmental effects, and/or human health effects.

The test data compiled for the category proves adequate to support a screening-level hazard assessment for the category and its members (CAS numbers, 88230-35-7, 90438-79-2, 108419-32-5, 108419-33-6, 108419-34-7, and 108419-35-8). One can assess the untested endpoints by extrapolation between and among the category anchor studies that adequately demonstrate the relatively low toxicity of the Alkyl Acetates C6 - C13.

The use of an Alkyl Acetate C6 - Cl3 category will inform the public earlier about any hazards of Alkyl Acetates C6 - C13. Second, the matrix of completed anchor study testing demonstrates the safety of the category without end-point tests for each chemical. Third, this reduction in testing will result in fewer animals used to test this category of chemicals as opposed to doing each test on individual Alkyl Acetates C6 - C13.

II. CHEMICAL PROCESS AND DESCRIPTION

The Alkyl Acetate C6 - Cl 3 category, for the purposes of the Challenge Program, is a group of Alkyl Acetates whose physicochemical and toxicological properties are very similar and follow a regular pattern as a result of synthesis and structural similarity (Table 1). The production of the alkyl acetate family involves the reaction of aliphatic, monohydric alcohols with acetic acid to form the corresponding acetate esters.

$$ROH + CH_3COOH \rightarrow CH_3COOR + H_2O$$

The structural similarities create a predictable pattern in the following parameters: physicochemical properties, environmental fate and environmental effects, and/or human health effects. The similarities are based on the following:

- A common structure - CH_3COOR,
- An incremental and constant change across the category where R is a branched alkyl group having carbon numbers of C6, C7, C8, C9, Cl 0, or Cl 3 as the main constituent,
- A common functional ester group, and
- A likelihood of common precursors and breakdown products which result in structurally similar chemicals (e.g., acetic acid and intermediate-chain aliphatic alcohols).

Table 1. CAS Numbers and Descriptions

CAS Number	Chemical Name	Generic Name
88230-35-7	Hexanol, acetate, branched and linear	C6 branched and linear alkyl acetate ester
90438-79-2	Acetic acid, C6-8 branched alkyl esters	C6-C8 branched alkyl acetate ester
108419-32-5	Acetic acid, C7-9 branched alkyl esters*	C7-C9 branched alkyl acetate ester
108419-33-6	Acetic acid, C8-10 branched alkyl esters*	C8-C10 branched alkyl acetate ester
108419-34-7	Acetic acid, C9-11 branched alkyl esters*	C9-C11 branched alkyl acetate ester
108419-35-8	Acetic acid, Cl l-14 branched alkyl esters	Cl l-Cl4 branched alkyl acetate ester

* = Not currently HPV but included to facilitate category evaluation

In formulating the category, Alkyl Acetates C6 - Cl 3, robust summaries of SIDS endpoints are addressed for the anchor alkyl acetate studies.

Category, Alkyl Acetates C6 - C13, accomplishes the goal of the Challenge Program - to obtain screening level hazard information - through the strategic application of testing across the category. The testing strategy results show that these chemicals behave in a similar or predictable manner and (1) extrapolation can be used to assess the Alkyl Acetates for which limited endpoint test data are available, and (2) no additional screening-level testing will be necessary. There will be a minimal amount of data modeling to be performed in 2001.

Procedures to assess the reliability of selected data for inclusion in the HPV Challenge Program were based on the guidelines described by Klimisch et al, 1997.

III. TEST PLAN RATIONALE

A. Physicochemical Data

Physicochemical data (i.e., melting point, boiling point, vapor pressure, water solubility, and Kow) for selected chemical components in the C6 - Cl3 Alkyl Acetate category will be calculated using the EPIWIN© model (EPIWIN, 1999), as discussed in the EPA document titled "The Use of Structure-Activitv Relationships (SAR) in the High Production Volume Chemicals Challenge Program." These data will be presented as ranges, based on the chemical components selected to represent each individual Alkyl Acetate product. In addition, measured data for some of these endpoints will also be

provided for selected Alkyl Acetate products where readily available. Where possible, the measured and calculated data will be presented together for comparison purposes. Table 2 lists selected measured physicochemical data as they appear on the material safety data sheets for these products and are provided with this test plan to further support considering these products a distinct category under the HPV Chemical program.

Table 2. Selected Physical Properties of Alkyl Acetates C6 - Cl3

CAS NUMBER	CHEMICAL NAME	BOILING RANGE (° C)	VAPOR PRESSURE (mm Hg @ 20° C)	SPECIFIC GRAVITY	FLASH POINT (° C)
88230-35-7	Hexanol, acetate, branched and linear	164-176	1.6	0.87	57
90438-79-2	Acetic acid, C6-8 branched alkyl esters	176-200	1.3	0.87	66
108419-32-5	Acetic acid, C7-9 branched alkyl esters	186-215	0.8	0.87	77
108419-33-a	Acetic acid, C8-10 branched alkyl esters	205-235	0.15	0.87	90
108419-34-7	Acetic acid, C9-11 branched alkyl esters	220-250	0.07	0.87	100
108419-35-8	Acetic acid, Cl 1-14 branched alkyl esters	240-285	0.04	0.87	127

B. Human Health Effects

The structural similarity of the Alkyl Acetates C6 - Cl3 influences both their physicochemical (Table 2) and their toxicological properties (Table 3). As a chemical category, the Alkyl Acetates C6 - C13, have predictable, low-level environmental and health hazards.

ExxonMobil Chemical Company believes the category of Alkyl Acetates C6 - Cl3 is scientifically justifiable and the test data compiled for the category proves adequate to support a screening-level hazard assessment for the category and its members (CAS numbers, 88230-35-7, 90438-79-2, 108419-32-5, 108419-33-6, 108419-34-7, and 108419-35-8). One can assess the untested endpoints by extrapolation between and among the category members.

The initial metabolic hydrolysis of the Alkyl Acetates results in reversal of the synthesis reaction. Metabolism of the Alkyl Acetates is catalyzed by esterases to yield acetic acid

and the corresponding aliphatic alcohol. Alcohol residues liberated by esterases, would likely be broken down by mitochondrial beta-oxidation or by cytochrome P450 mediated omega and omega-minus-one oxidation (may be followed by beta-oxidation). The alcohol undergoes various oxidative steps to yield other alcohols, ketones, aldehydes, carboxylic acids and carbon dioxide (Mann, 1987). Because alcohols are the primary metabolites of Alkyl Acetates, data on alcohols are very useful to address the toxicologic properties of Alkyl Acetates. Data for monohydric, aliphatic alcohols show a systematic variation according to molecular weight in a manner similar to many other homologous series (Monick, 1968). The body handles aliphatic hydrocarbons in a similar manner via oxidative conversion to alcohols, ketones, and eventual elimination as carbon dioxide and carboxylic acids (Wislocki et al, 1980). The undegraded alcohols can be conjugated either directly or as a metabolite with glucuronic acid, sulfuric acid, or glycine and are rapidly excreted (Lington and Bevan, 1994). Acetyl residues liberated by the esterases would enter intermediary metabolism pathways, be broken down and excreted as carbon dioxide and water. Intermediate aldehydes could be reactive and bind with DNA and/or proteins. Glucuronidation and glutathione conjugation are possible means of rapid elimination (Mann, 1987).

Table 3. Alkyl Acetates C6 - Cl3 Data Matrix For Mammalian Toxicity Studies

CAS Number	88230- 35-7	90438-79-2	108419-32-5	108419-33-6	108419-34-7	108419-35-8
Branched Alkyl Acetate Ester	C6	C6-C8	C7-C9	C8-C10	C9-C11	C11-C14
ACUTE						
ORAL -RAT	XX	R	R	R	R	x x
DERMAL - RABBIT	xx	xx	xx	xx	xx	xx
GENOTOXICITY						
Genetic - Point Mutation	xx	xx	xx	RA	RA	x x
Genetic - Chromosome Aberration	xx	xx	xx	RA	RA	xx
REPEATED DOSE						
ORAL - Rat	xx 28-DAY Gavage	RA	xx OO-DAY Gavage	RA	RA	xx 90-DAY Gavage
REPRODUCTIVE I DEVELOPMENTAL						
Developmental Tox ORAL - Rat	RA	RA	x x	RA	RA	x x
Reproductive Tox	Read across to Developmental Toxicity Studies and Repeated Dose Toxicity Studies that included histopathology on male and female sex organs and accessory sex organs.					

XX Anchor Studies with Adequate Existing Data; Studies are reliable without restrictions (Robust Summaries presented).
RA Read Across Extrapolation.
R Referenced Supportive Internal Study Document (No Robust Summary Provided).

Table 4. Summary of Toxicology Data Endpoints for Alkyl Acetates C6 - Cl3 Anchor Studies

NAME	ORAL LD_{50} -RAT	DERMAL LD_{50} - RABBIT	ORAL REPEATED DOSE - Rat	DEVELOPMENT - Rat	AMES Test ± Activation	CHROMOSOMAL ABERRATION - In Vitro or In Vivo
Hexanol, acetate, branched and linear	>2 glkg and >10 g/kg	>2 g/kg and >3.16 g/kg	28-DAY Gavage NOAEL = 1000 mglkglday	RA	NEGATIVE	NEGATIVE CHROM ABS (CHO)
Acetic acid, C6-8 branched alkyl esters	>5 g/kg *	>3.16 g/kg	RA	RA	NEGATIVE	NEGATIVE CHROM ABS (CHO)
Acetic acid, C7-9 branched alkyl esters*	>5 glkg *	>3.16 g/kg	90-DAY Gavage NOAEL = 1000 mglkglday	DEV-TOX MATERNAL NOAEL = 500 mg/kg; PUP NOAEL = 500 mg/kg	NEGATIVE	INACTIVE CD-I MOUSE MICRO-NUCLEUS
Acetic acid, C8-10 branched alkyl esters*	>5 g/kg *	>3.16 g/kg	RA	RA	RA	RA
Acetic acid, C9-11 branched alkyl esters*	>5 g/kg *	>3.16 g/kg	RA	RA	RA	RA
Acetic acid, CII-14 branched alkyl esters	>5 g/kg	>3.16 g/kg	90-DAY Gavage NOAEL = 1000 mg/kg/day	DEV-TOX MATERNAL NOAEL = 500 mg/kg; PUP NOAEL = 2 5 0 0 mg/kg	NEGATIVE	INACTIVE CD-1 MOUSE MICRO-NUCLEUS

RA Read Across.
* Referenced Supportive Internal Study Document (No Robust Summary Provided)

C. Presentation of Alkyl Acetates C6 - Cl3 Category Data Associated with the Anchor Studies under the HPV Challenge Program

Acute Oral Toxicity

TEST	C6 branched and linear alkyl acetate ester	C6-C8 branched alkyl acetate ester	C7-C9 branched alkyl acetate ester	C8-C10 branched alkyl acetate ester	C9-C11 branched alkyl acetate ester	C11-C14 branched alkyl acetate ester
ACUTE ORAL - RAT	LD_{50}>10 g/kg (HL, 1963) LD_{50}>2 g/kg (EBSI, 1995a)	LD_{50}>5 g/kg (Biodyn, 1983a) *	LD_{50}>5 glkg (Biodyn, 1984a,) *	LD_{50}>5 g/kg (Biodyn, 1983b) *	LD_{50}>5 g/kg (Biodyn, 1983c) *	LD_{50}>5 g/kg (Biodyn. 1983d)

* References] Supportive Internal Study Document (No Robust summary Provi d)

All of the Alkyl Acetates C6 - Cl3 have a low order of toxicity via the oral route of exposure to rats. The LD_{50} for C6 branched and linear alkyl acetate ester anchor studies were >2 to >10 g/kg (EBSI, 1995a; HL, 1963; ~~EBSI 1 99~~%). The LD_{50} for Cl l-Cl4 branched alkyl acetate ester anchor study was greater than 5 g/kg (Biodyn, 1983d). The LD_{50}'s for the referenced supportive C6-C8, C7-C9, C8-Cl 0, and C9-C11 branched alkyl acetate esters were all > 5 g/kg (Biodyn, 1983a;

1984a; 1983b; 1983c). No evidence of systemic toxicity was seen in any of these studies.

Acute Dermal Toxicity

TEST	C 6 branched and linear alkyl acetate ester	C6-C8 branched alkyl acetate ester	C7-C9 branched alkyl acetate ester	C8-C10 branched al kyl acetate ester	CQ-Cl1 branched alkyl acetate ester	C11-C14 branched alkyl acetate ester
ACUTE DERMAL - RABBIT	LD_{50}>3.16 g/kg (HL,1963) LD_{50}>2 g/kg (EBSI, 1995b)	LD_{50}>3.16 g/kg (Biodyn, 1983e)	LD_{50}>3.16 g/kg (Biodyn, 1983f)	LD_{50}>3.16 g/kg (Biodyn, 1983g)	LD_{50}>3.16 g/kg (Biodyn, 1964b)	LD_{50}>3.16 g/kg (Biodyn, 1984c)

The Alkyl Acetates C6 - Cl 3 have a low order of toxicity via the dermal route of exposure. The rabbit dermal LD_{50} for the C6 branched and linear alkyl acetate ester anchor study was greater than 2 or 3.16 g/kg (EBSI, 1995b; HL, 1963). The rabbit dermal LD_{50} for Cl l-Cl4 branched alkyl acetate ester anchor study was greater than 3.16 g/kg (Biodyn, 1984c). The rabbit dermal LD_{50}'s for the C6-C8, C7-C9, C8-C10, and C9-C11 branched alkyl acetate esters were also greater than 3.16 g/kg (Biodyn, 1983e; 1983f; 1983g; 1984b).

Genotoxicity

TEST	C6 branched and linear alkyl acetate ester	C6-C8 branched alkyl acetate ester	C7-C9 branched alkyl acetate ester	C8-C10 branched alkyl acetate ester	C9-C11 branched alkyl acetate ester	C11-C14 branched alkyl acetate ester
AMES - S. typhimurium; TA98, 100, 1535, 1537.1538 ± Activation	NEGATIVE (EBSI, 1995c)	NEGATIVE (EBSI, 1997a)	NEGATIVE (EBSI, 1994a)	RA	RA	NEGATIVE (EBSI, 1994b)
Chromosomal Aberration - In Vitro or In Vivo	NEGATIVE CHROM ABS (CHO) (EBSI, 1995d)	NEGATIVE CHROM ABS (CHO) (EBSI, 1997b)	INACTIVE CD-I MOUSE MICRO-NUCLEUS (EBSI, 1994c)	RA	RA	INACTIVE CD-I MOUSE MICRO-NUCLEUS (EBSI, 1994d)

RA Read Across

The Alkyl Acetates C6 - Cl3 have shown no evidence of genotoxicity. Neither of the anchor studies, the C6 branched and linear alkyl acetate ester nor the Cl 1-Cl4 branched alkyl acetate ester were mutagenic in Ames assays using five strains of *Salmonella typhimurium*, with and without metabolic activation (EBSI, 199%; 1994b). The C6-C8 and C7-C9 branched alkyl acetate ester assays likewise were negative in the Ames assays (EBSI, 1997a; 1994a).

The clastogenicity of the anchor study, C6 branched and linear alkyl acetate ester was investigated in an in vitro chromosomal aberration assay in CHO cells

and was negative (EBSI, 1995d) as was the C6-C8 branched alkyl acetate ester study (EBSI, 1997b).

The clastogenicity of the Cl l-Cl4 branched alkyl acetate ester anchor study was investigated in the *in vivo* mouse micronucleus assay and was inactive for producing an increase in micronuclei formation in the bone marrow of CD-l mice (EBSI, 19944) as was the C7-C9 branched alkyl acetate ester study (EBSI, 1994c). Both mouse micronucleus assays showed evidence of cytotoxicity at the highest doses as shown by a decrease in the percentage of polychromatic erythrocytes compared to negative controls (EBSI, 1994c; EBSI, 19944).

Subchronic Toxicity

TEST	C6 branched and linear alkyl acetate ester	C7-C9 branched alkyl acetate ester	Cl 1 -C14 branched alkyl acetate ester
ORAL - Rat	28-DAY Gavage NOAEL = 1000 mglkglday (EBSI, 1995e)	OO-DAY Gavage NOAEL = 1000 mg/kg/day; NOEL = 100 mglkglday (Biodyn. 1985a)	OO-DAY Gavage NOAEL = 1000 mg/kg/day; NOEL = 100 mg/kg/day (Biodyn, 1985b)

An evaluation of the repeated dose anchor studies indicates a low toxicity concern for Alkyl Acetates C6 - Cl 3. Rats were exposed to 0, 100, 500 or 1000 mg/kg/day C6 branched and linear alkyl acetate ester for 28 days. No clinical signs of toxicity were observed at any time during the study. All animals survived to study termination and there were no treatment-related clinical, in-life, gross postmortem or microscopic findings (including adrenal glands, heart, kidneys, liver, lung, spleen, testes and ovaries). There were no adverse effects on body weight, food consumption, clinical laboratory parameters or organ weights. The no observable adverse effect level (NOAEL) was 1000 mglkglday (EBSI, 1995e).

A 90-day oral subchronic study was conducted in Sprague-Dawley rats with C7-C9 branched alkyl acetate ester at doses of 100, 500, and 1000 mg/kg of body weight administered by gavage. Liver weights were elevated at the 45-day interim sacrifice. Terminal liver and kidney weights were elevated in a dose-related manner. Organ weight changes were generally considered to be adaptive changes and did not indicate toxic effects. There were no abnormal necropsy observations or elevated serum chemistry values; thus, these increased organ weights were not treatment related. Microscopic evaluation of the kidneys revealed evidence of mild tubular nephropathy only in high-dose male rats that were consistent with alpha-2-u-globulin effects. Histopathology review of all other tissues from high-dose animals, including reproductive organs (testes, epididymides, prostate, seminal vesicles, ovaries, uterine horns, cervix, corpus of the uterus, and vagina) showed normal morphology. The lowest observable effect level was 500 mg/kg (increased liver/body weight ratio); however this is of minimal toxicological significance. The no observable adverse effect level (NOAEL) was 1000 mg/kg (Biodyn, 1985a).

A 90-day oral subchronic study was conducted in rats with Cl l-Cl4 branched alkyl acetate ester at doses of 100, 500, and 1000 mg/kg of body weight

administered by gavage. Terminal liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and do not indicate toxic effects. Microscopic evaluation of the kidneys revealed evidence of mild tubular nephropathy only in the high-dose male rats that was consistent with alpha-2-u-globulin effects not expected to occur in humans. Histopathology review of all other tissues from high-dose animals, including reproductive organs (testes, epididymides, prostate, seminal vesicles, ovaries, uterine horns, cervix, corpus of the uterus, and vagina) showed normal morphology. The no observable adverse effect level (NOAEL) was 1000 mglkg. (Biodyn, 1985b).

Developmental Toxicity

TEST	C7-C9 branched alkyl acetate ester	Cl 1 -C14 branched alkyl acetate ester
ORAL - Rat	DEV-TOX MATERNAL NOEL = 100 mglkg; PUP NOEL = 500 mglkg (Biodyn, 1985c)	DEV-TOX MATERNAL NOEL = 500 mg/kg; PUP NOEL = 2500 mglkg (Biodyn, 1985d)

The Alkyl Acetates C6 - Cl 3 anchor study products evaluated for developmental toxicity were C7-C9 and Cl l-Cl4 branched alkyl acetate ester. The C7-C9 branched alkyl acetate ester was administered at 100, 500, and 1000 mg/kg on gestation days 6-l 5 in a developmental toxicity study in rats. Maternal toxicity was seen at mid and high doses as evidenced by decreases in body weight. There was a slight increase in fetal malformations and embryotoxicity in the high-dose group only; no adverse fetal effects were observed in the mid- or low-dose groups. A maternal NOEL of 100 mg/kg and a developmental NOEL of 500 mg/kg were observed (Biodyn, 198%).

The Cl 1 -Cl4 branched alkyl acetate ester was administered at 500, 1300, and 2500 mg/kg on gestation days 6-l 5 in a developmental toxicity study in rats. Maternal toxicity was seen at mid and high doses as evidenced by decreases in body weight. There were no statistically significant deleterious effects on fetal survival, body weight, crown-rump length and no evidence of treatment-related malformations. A maternal NOAEL of 500 mg/kg and a developmental NOAEL of 2500 mglkg were observed (Biodyn, 1985d).

Reproductive Toxicity

The three repeated dose toxicity anchor studies (C6 branched and linear alkyl acetate ester, and C7-C9, Cl l-Cl4 branched alkyl acetate ester) and the two developmental toxicity anchor studies (C7-C9 and Cl 1-C14 branched alkyl acetate ester) prove adequate to support a screening-level hazard assessment for reproductive toxicity for Alkyl Acetates C6 - C13. This conclusion is based on the organ weights (ovaries and testes), gross and microscopic histopathology observations that showed the male and female sex organs and accessory sex organs were with in normal control ranges. There were no treatment-related histopathologic effects in the reproductive organs for any test animals in the repeated dose or developmental toxicity studies. According to the OECD SIDS

Guidelines, adequate developmental toxicology data coupled with subchronic toxicity data showing no effects on reproductive organs, fulfills the reproductive endpoint.

D. Aquatic Toxicity

Products ranging from the C6 branched and linear alkyl acetate ester to C9-C11 branched alkyl acetate ester are expected to produce a relatively narrow range of moderate acute aquatic toxicity to freshwater fish and invertebrates, and a similar narrow range of moderate toxicity to freshwater algae. This is based on results of studies for selected products in this range of alkyl acetate esters. In comparison, the Cl 1-C14 branched alkyl acetate is not expected to produce acute aquatic toxicity to freshwater fish and invertebrates, or toxicity to freshwater algae, based on results of studies for this product. The lack of toxicity is due to its comparatively lower water solubility, which limits the exposure of aquatic organisms to soluble fractions of this product.

Fish Acute Toxicity

TEST	C 6 branched and linear alkyl acetate ester	C6-C8 branched alkyl acetate ester	C7-C9 branched alkyl acetate ester	C8-C10 Branched alkyl acetate ester	C9-C11 branched alkyl acetate ester	C11-C14 branched alkyl acetate ester
FISH ACUTE TOXICITY (96-hour)	LL_{50}= 11.9 mg/L (EBSI, 1995f)	LC_{50}= 8.2 mg/L (EBSI, 1997c)	LC_{50}= 14.9 mg/L* (EBSI, 1985a)	RA	RA	LL_0= 5800 mg/L (EBSI, 1985b)

RA read across
* based on total carbon analysis

Acute experimental toxicity tests are reported for rainbow trout (*Oncorhynchus mykiss*) and fathead minnow (*Pimephales promelas*). Experimental values for C6 branched and linear alkyl acetate ester, C6-C8 branched alkyl acetate ester, and C7-C9 branched alkyl acetate ester show that they have the potential to cause acute toxicity (96-hour LL50 or LC50) in a range of approximately 8 to 15 mg/L. Although there are no data for C8-C10 branched alkyl acetate ester or C9-C11 branched alkyl acetate ester, their acute toxicities are expected to be similar to the existing fish acute toxicity data based on invertebrate acute toxicity test results, which show that these 5 products demonstrate a relatively narrow range of acute toxicity. In comparison, no mortality was observed with a fathead minnow when exposed to a saturated solution of a Cl l-Cl4 branched alkyl acetate ester prepared at a test material loading of 5800 mg/L.

Invertebrate Acute Toxicity

TEST	C 6 branched and linear alkyl acetate ester	C6-C8 branched alkyl acetate ester	C7-C9 branched alkyl acetate ester	C8-C10 branched alkyl acetate ester	C9-C11 branched alkyl acetate ester	CII-CI4 branched al kyl acetate ester

TEST	C6 branched and linear alkyl acetate ester	C6-C8 branched alkyl acetate ester	C7-C9 branched alkyl acetate ester	C8-C10 branched alkyl acetate ester	C9-C11 branched alkyl acetate ester	C11-C14 branched alkyl acetate ester
DAPHNID ACUTE TOXICITY (48-hour)	EL_{50}= 7.6 mg/L (EBSI, 1995g)	RA	EC_{50}= 29.4 mg/L* (EBSI, 1985c)	RA	EL_{50}= 6.7 mg/L (EBSI, 2000)	EL_0= 5829 mg/L (EBSI, 1985d)

RA read across
* based on total carbon analysis

Acute experimental toxicity tests for three alkyl acetate esters are reported for a Daphnid (*Daphnia* magna). The results show that these products have the potential to cause acute toxicity (48-hour EL50 or EC50) in a range of approximately 7 to 30 mg/L. In comparison, no effect was observed with the same organism exposed to a saturated solution of a Cl l-Cl4 branched alkyl acetate ester prepared at a test material loading of 5829 mg/L.

Alga Toxicity

TEST	C 6 branched and linear alkyl acetate ester	C6-C8 branched alkyl acetate ester	C7-C9 branched alkyl acetate ester	C8-C10 branched alkyl acetate ester	C9-C11 branched alkyl acetate ester	C11-C14 branched alkyl acetate ester
ALGA TOXICITY (96-hour)	EL_{50}b(1) = 40.1 mg/L; EL_{50}gr(2)= 32.1 mg/L; NOELRb= 31.0 mg/L; NOELRgr= 8.0 mg/L (EBSI, 1995h)	RA	EL_{50}b = 19.4 mg/L*; EL_{50}gr = 43.5 mg/L*; NOELRb= 31.0 mg/L*; NOELRgr= 8.0 mg/L* (EBSI, 1985e; EBSI, 1994e)	RA	RA	EL_0b = 5829 mg/L; EL0gr = 5829 mg/L; NOELRb= 5829 mg/L; NOELRgr= 5829 mg/L (EBSI, 1985f)

(1) biomass
(2) growth rate
RA read across
* based on total carbon analysis

Acute experimental toxicity tests are reported for an alga (*Selenastrum capricornutum*). Experimental values for C6 branched and linear alkyl acetate ester and C6-C8 branched alkyl acetate ester show that these products have the potential to cause acute toxicity (96-hour EL50 for biomass, b, and growth rate, gr) in a range of approximately 19 to 44 mg/L. Although there are no data for C6-C8 branched alkyl acetate ester, C8-Cl 0 branched alkyl acetate ester, or C9-C11 branched alkyl acetate ester, their acute toxicities are expected to be similar to the existing alga acute toxicity data based on invertebrate acute toxicity test results, which show that these 5 products demonstrate a relatively narrow range of acute toxicity. In comparison, no effect on biomass or growth rate was observed with the same organism when exposed to a saturated solution of a Cl l-Cl4 branched alkyl acetate ester prepared at a test material loading of 5829 mg/L.

E. Environmental Fate

Biodegradation data are available for four alkyl acetate ester products, which show that with the exception of the highest molecular weight product, these ester products are rapidly biodegraded. The Cl 1-C14 branched alkyl acetate ester has been shown to biodegrade at a moderate rate, which suggests that although it is not expected to degrade at a rate equivalent to the lighter molecular weight alkyl acetate ester products, it also will not persist in the environment.

Hydrolysis data developed for two alkyl acetate ester products suggest that the entire range of alkyl acetate ester products is stable in water. Although there is some information on photodegradation and fugacity, a complete data set will be developed to adequately characterize the alkyl acetate ester products. Chemical equilibrium models are used to calculate fugacity, which describes the potential of a chemical to be distributed in the environment. These data can only be calculated. Available information for selected component chemicals in the alkyl acetate ester category suggests that these products are expected to partition primarily to the air. Therefore, their fate in air is of environmental interest (this is discussed below under photodegradation). In addition, the majority of the component chemicals in these products have relatively low Kow values, which suggests that they will not tend to partition to suspended organic matter in air and precipitate to aquatic and terrestrial environmental compartments.

Biodegradation

TEST	C 6 branched and linear alkyl acetate ester	C6-C8 branched alkyl acetate ester	C7-C9 Branched alkyl acetate ester	C8-C10 branched alkyl acetate ester	C9-C11 branched alkyl acetate ester	CII-CI4 branched alkyl acetate ester
28-Day Aerobic Biodegradation Test	76.9% (EBSI, 1994f)	77.1% (EBSI, 1998)	RA	RA	84.7% (EBSI, 1996)	31.0%* (EBSI, 1985g)

RA read across
• data developed using an acclimated inoculum

C6 branched and linear alkyl acetate ester, C6-C8 branched alkyl acetate ester, and C9-C11 branched alkyl acetate ester have been shown to biodegrade rapidly using 28-day standard biodegradation test procedures. In comparison, Cl l-Cl4 branched alkyl acetate ester biodegrades at a moderate rate, which suggests that although it is not expected to degrade at a rate equivalent to the lighter alkyl acetate ester products, it will not persist in the environment.

Upon review of the available information, sufficient quality data were identified to accurately characterize the biodegradability of the products in this category, The data show that all products except the Cl l-Cl4 branched alkyl acetate ester are expected to biodegrade to an extent ranging from approximately 77 to 85% after 28 days. These data were developed using non acclimated inocula. The tests used various closed systems, which is required when assessing the biodegradability of volatile materials like

those in this category. The test systems were continuously stirred, which is also recommended when evaluating mixtures containing several chemicals, some of which may have minimal water-solubility. In comparison, the Cl l-Cl4 branched alkyl acetate ester demonstrated a lower extent of biodegradability, 31%, using an acclimated inoculum after the same period of time.

Photodegradation - Photolysis

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may undergo a transformation. Simple chemical structures can be examined to determine whether a chemical has the potential for direct photolysis in water. First order reaction rates can be calculated for some chemicals that have a potential for direct photolysis using the procedures of Zepp and Cline (Zepp, 1977). UV light absorption of the chemical components in this category will be evaluated to identify those having the potential to degrade in solution. For those compounds with a potential for direct photolysis in water, first order reaction rates will be calculated.

Photodegradation - Atmospheric Oxidation

Photodegradation can be measured (US EPA, 1999a) (EPA identifies OECD test guideline 113 as a test method) or estimated using models accepted by the EPA (US EPA, 1999b). An estimation method accepted by the EPA includes the calculation of atmospheric oxidation potential (AOP). Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation, but rather indirect degradation. AOPs can be calculated using a computer model. Alkyl Acetates, such as those in the Alkyl Acetate category, have the potential to volatilize to air. In air, these chemicals may undergo reaction with photosensitized oxygen in the form of ozone and hydroxyl radicals. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPIWIN, 1999) is used by OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall OH reaction rate constant, a 12-hr day, and a given OH- concentration. This calculation will be performed for the representative chemical components in the alkyl acetate ester category.

Stability in Water (Hydrolysis)

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). Stability in water can be measured (US EPA, 1999a) (EPA identifies OECD test guideline 111 as a test method) or estimated using models accepted by the EPA (US EPA, 199913).

Upon review of the available information, sufficient quality data were identified to accurately characterize the hydrolysis potential of the products in this category. Results of two studies for the C6 branched and linear alkyl acetate ester and C6-C8 branched

alkyl acetate ester products indicate that these products are stable in water and are not subject to physically mediated hydrolysis at environmentally relevant pH values and over environmentally relevant time periods (EBSI, 1995i; EBSI, 1995j).

Chemical Transport and Distribution In The Environment (Fugacity Modeling)

Fugacity based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The US EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model (Mackay, 1996). EPA cites the use of this model in its document titled *Determining the Adequacy of Existing Data* (US EPA, 1999a), which was prepared as guidance for the HPV Program.

In its document, EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 6 compartments (air, soil, water, suspended sediment, sediment, biota) within a unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. This model will be used to calculate distribution values for representative chemical components identified in products in this category. A computer model, EPIWIN – version 3.02 (EPIWIN, 1999), will be used to calculate the properties needed to run the Level I EQC model.

IV. TEST PLAN SUMMARY

ExxonMobil Chemical believes that the Alkyl Acetate C6 - Cl 3 category of chemicals should be further examined in the following manner:

- Calculate physicochemical data as described in the EPA document titled, *The Use of Structure-Activify Relationships (SAR)* **in** *the High Production Volume Chemicals Challenge Program* for selected chemical components of Alkyl Acetate products in this category. Provide measured data for selected products where readily available.
- Prepare a technical discussion on the potential of Alkyl Acetate products in this category to photodegrade. Calculate AOP values for selected chemical components of alkyl acetate ester products in this category.
- Calculate fugacity data for selected chemical components of alkyl acetate ester products in this category.

ExxonMobil Chemical believes that the Alkyl Acetate C6 - Cl3 category of chemicals should be exempt from additional animal testing based on:

- available toxicologic data on Alkyl Acetates,
- established metabolic pathways for Alkyl Acetates,
- available toxicologic data on alkyl acetate metabolites, and
- well established structure-activity relationships.

ExxonMobil Chemical Company believes the thorough evaluation of the strategic anchor studies and the overall robustness of the screening data set for an Alkyl Acetates C6 - Cl3 category complies with the objectives of the HPV volunteer testing program. The category is supported by the basic data assessment of the physicochemical properties, environmental fate, and human and environmental effects of chemicals as defined by the Organization for Economic Cooperation and Development (OECD).

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Acute Oral Toxicity

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	Experimental (Non-regulatory)
Type	LD50
GLP	Pre-GLP
Year	1963
Species/Strain	Rat - Sprague-Dawley
Sex	Male
#/sex/dose	5
Vehicle	Corn oil (1 .O % or IO % v/v)
Route of Admin	Oral Gavage
Doses	34.6, 120,417, 1450, 5000, or 10,000 mg/kg
• **Dose/time**	Single dose following 3-4 hour-fast
• **Post Dose Observation Period**	1, 4, and 24 hours postdosing and daily for 14 Days
Results	
. **LD50**	>1 0 g/kg
• **Remarks**	One animal at the 1450 mg/kg dose level died on day 11. No toxic signs were observed prior to death and a normal body weight-gain was recorded at death. Postmortem examination showed congestion of the lungs, kidneys, adrenals, and pancreas, and gaseous distention of the stomach and large intestine at the time of death. All other animals showed no gross pathology following termination. Principal toxic effects seen only at the 10,000 mg/kg dose were depression, ataxia, sprawling of limbs and depressed righting reflex only at the 24-hour observation.
• **Conclusion**	The acute oral LD50 for C6 branched and linear alkyl acetate ester in male Sprague-Dawley rats is >1 0 g/kg.
Data Quality	1 - Reliable study without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Hazleton Laboratories Incorporated, Falls Church, VA, USA, Project # 38355.

Acute Oral Toxicity

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	Experimental (EU Annex V, B.1 and OECD 401)
Type	Limit
GLP	Yes
Year	1995
Species/Strain	Rat - Crl:CDBR
Sex	Male & Female
#/sex/dose	5
Vehicle	None
Route of Admin	Oral Gavage
Doses	2000 mg/kg
• **Doses/time**	Single
• **Post Dose Observation Period**	14 Days
Results	
. **LD50**	>2 g/kg
• **Remarks**	There was one female death on Day 0 at the 2-hour observation considered to be the result of test material aspiration during dosing. Clinical signs of toxicity were limited to nasal, oral and/or ocular discharge, abdominal and/or anogenital staining, and/or soft stool in four males at the Day 0 interval. One male and 4 females were free of abnormalities during the entire study. No gross abnormalities were seen at postmortem examination.
• **Conclusion**	C6 branched and linear alkyl acetate ester, did not elicit signs of acute systemic toxicity when administered orally. Signs of slight toxicity (staining of the fur and soft stool) were limited to the male animals on Day 0. There was one female death on Day 0, but the death was the result of test material aspiration, not toxicity.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, Acute Oral Toxicity Test in the Rat; Project # 101501.

Acute Dermal Toxicity

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	Experimental (Non-regulatory)
Type	Limit
GLP	Pre-GLP
Year	1963
Species/Strain	Rabbit (albino)
Sex	Male & Female
#/sex/dose	1
Vehicle	None
Route of Admin	Dermal Application
Doses	50, 200, 794 or 3160 mg/kg
• **Doses/time**	Single application / 24-Hour Occlusive Patch
• **Post Dose Observation Period**	14 Days
Results	
. **LD50**	>3.16 glkg
• **Remarks**	Two animals, 200 and 3160 mg/kg dosage levels, showed soft feces or diarrhea for two to four days. One animal, 794 mg/kg dosage level, showed diarrhea during the second week and weight loss at termination. All other animals were normal and showed body weight gains. There were no gross pathological findings at the study termination.
• **Conclusion**	C6 branched and linear alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Hazleton Laboratories, Inc., Falls Church, VA, USA; Project # 38355.

Acute Dermal Toxicity

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	Experimental (EU Annex V, 8.3; OECD 402)
Type	Limit
GLP	Yes
Year	1995
Species/Strain	Rabbit - New Zealand White
Sex	Male & Female
#/sex/dose	5
Vehicle	None
Route of Admin	Dermal
Doses	2000 mg/kg
• **Doses/time**	Single application / 24-Hour Occlusive Patch
• **Post Dose Observation Period**	14 Days
Results	
. **LD50**	>2 glkg
• **Remarks**	There were no signs of systemic toxicity. Slight dermal irritation was noted in all animals, with the most severe response being observed at the Day 1 observation interval. At post mortem examination, all animals had desquamation at the dose site. In general, dermal responses were considered minimal and transient in nature.
• **Conclusion**	C6 branched and linear alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, Acute Dermal Toxicity Study in the Rabbit; Project # 101506.

Genetic Tox *In Vitro*

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	EU Annex V, 8.14; OECD 471
Type	Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)
System of Testing	Bacterial
GLP	Yes
Year	1995
Species/Strain	S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538
Metabolic Activation	
• **Species/cell type**	Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9)
Concentrations Tested	250, 500, 1000, 2000, and 3000 µg/plate
Vehicle	DMSO
Remarks for Test Conditions	There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 250, 500, 1000, 2000, and 3000 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37 ± 2 °C for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.

Results

- **Remarks**

C6 branched and linear alkyl acetate ester, did not induce significant increases in revertant colonies (≥ 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains.

Toxicity was observed in both the initial and repeat assays in the following strains and dose levels: TA96 at 2000 µg/plate without metabolic activation, and at 3000 µg/plate with and without metabolic activation; TA100 at 2000 and 3000 µg/plate with and without metabolic activation; TA1535 at 2000 µg/plate without metabolic activation; TA1 537 at 250, 500, 1000, 2000, and 3000 µg/plate without metabolic activation; and TA1 538 at 1000 and 2000 µg/plate without metabolic activation, and at 3000 µg/plate with and without metabolic activation. The nontreated and vehicle controls responded in a manner consistent with data from previous assays.

- **Conclusion**

C6 branched and linear alkyl acetate ester was not mutagenic in any strain of Salmonella typhimurium tested, but was toxic in all strains tested under the conditions of this study.

Data Quality

1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Assay; Project # 101525.

Genetic Tox *In Vitro*

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	*88230-35-7*
Method	Galloway, et al, *Development of a standard protocol for in vitro cytogenetic testing with Chinese hamster ovary cells: comparison of results for 22 compounds in two laboratories.* Environ. Mutagen. 7:1-*51, 1985.*
Type	In Vitro Chromosomal Aberration Assay in CHO Cells
System of Testing	Cultured Chinese hamster ovary (CHO) cells
GLP	Yes
Year	1995
Remarks for Test Conditions	Treatment group doses (14 total in initial and repeat assays) ranged from ***250-480*** μg/mL in the 20-hour initial test; 230-550 μg/mL in the 20- and 44-hour repeat assays. S9 activation was used in doses ranging from 350-480 μg/mL in the 20-hour initial assay and ranging from 380-550 μg/mL in the 20- and 44-hour repeat assays. Vehicle in all assays was DMSO (not exceeding 1.0% final volume to ensure normal cell viability and growth rate). Positive controls, N-methyl-N-Nitro-N-Nitrosoguanidine (MNNG - clastogen that does not require metabolic activation) and 7,12-Dimethylbenz[a]anthracene (DMBA- clastogen that requires metabolic activation) were used as positive controls in the nonactivated series and activated series, respectively.
Results	C6 branched and linear alkyl acetate ester, was tested in a 20-hour chromosome aberration assay using Chinese hamster ovary cells with and without metabolic activation. A repeat assay was also performed using 20-hour and 44-hour harvests. For the initial 20-hour harvest data, there was no evidence of a positive dose response nor of any treated group being different from the control in these analyses. For the repeat harvest, the high dose group (550 μg/mL) was statistically different from the vehicle control ($p<0.05$). However, this statistically significant finding (6.5% aberrant cells) was not reproducible. No increase was observed at the 44-hour harvest time. In addition, no increase was observed in the initial assay with metabolic activation at similar dose levels. There was no statistically significant finding in the 44-hour harvest.
Remarks	C6 branched and linear alkyl acetate ester, reduced cell survival by at least 50% when compared to the vehicle control in the repeat assay: 20-hour harvest without activation and 44-hour harvest with and without metabolic activation. All negative and positive controls used in this study performed in an appropriate manner.

Conclusion	C6 branched and linear alkyl acetate ester was considered negative for inducing chromosome aberrations under the conditions of this test at doses up to 550 μg/mL with and 430 μg/mL without metabolic activation.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, In Vitro Chromosomal Aberration Assav in CHO Cells, Project # 101532.

Repeated Dose Oral Toxicity

Test Substance	C6 branched and linear alkyl acetate ester
CAS #	88230-35-7
Method	EU Annex V, 8.7; OECD 407
Type	28-Day Repeated Dose Oral Toxicity
GLP	Yes
Year	1995
Species/Strain	Rat - Crl:CD BR
Sex	Male & Female
#/sex/dose	5
Vehicle	Corn Oil
Route of Admin	Gavage
Duration of Test	28-Day
Doses	0, 100, 500, and 1000 mg/kg/day
• **Volume**	5 ml/kg
Results	
. **NOAEL**	1000 mg/kg/day
• **Conclusion**	Oral administration of C6 branched and linear alkyl acetate ester daily to rats for 28 days did not produce any signs of overt systemic toxicity at any dose level tested. There were no treatment-related clinical in-life, gross postmortem or microscopic findings (including adrenal glands, heart, kidneys, liver, lung, spleen, testes and ovaries); no treatment-related mortality; and no adverse effects on body weight, food consumption, clinical laboratory parameters, or organ weights.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that affected the quality or integrity of the data.
Reference	Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, 28-Day Repeated Dose Oral Toxicity Study in the Rat; Project # 101570.

Acute Dermal Toxicity

Test Substance	C6-C8 branched alkyl acetate ester
CAS #	90438-79-2
Method	Experimental (Non-regulatory)
Type	Limit
GLP	Compliant
Year	1983
Species/Strain	Rabbit (New Zealand White)
Sex	Male & Female
#/sex/dose	3
Vehicle	None
Route of Admin	Dermal Application
Doses	3160 mg/kg
• **Doses/time**	Single application / 24-Hour Occlusive Patch
• **Post Dose Observation Period**	14 Days

Results

• **LD50**	>3.16 g/kg
• **Remarks**	There were no overt signs of systemic toxicity. Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14. Erythema was noted in all animals at 24 hours, ranging from moderate to severe, and regressed in all animals throughout the study. On Day 14, five of six animals showed very slight erythema and one had no signs of erythema. Edema was evident in all but one animal at 24 hours and by Day 14 all but one animal was free of signs of edema. Desquamation was evident in five animals on Day 14. All animals survived to termination of the study and increased in body weight. There were no significant findings at the postmortem gross examination.
• **Conclusion**	C6-C8 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Bio/dynamics Inc., East Millstone, NJ, USA, Acute Dermal Toxicity Study in the Rabbit with C6-C8 Branched Alkyl Acetate Ester. Project # 321106.

Genetic Tox *In Vitro*

Test Substance	C6-C8 branched alkyl acetate ester
CAS #	**90438-79-2**
Method	EU Annex V, B.14; OECD 471
Type	Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)
System of Testing	Bacterial
GLP	**Yes**
Year	1997
Species/Strain	S. typhimurium / TA98, TAIOO, TA1 535, TA1 537, TA1538
Metabolic Activation	
• **Species/cell type**	Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9)
Concentrations Tested	50, 100, 200, 400, 600, and 800 µg/plate (_ repeat assay only; ___ initial assay only)
Vehicle	DMSO
Remarks for Test Conditions	There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TAIOO, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 100, 200, 400, 600, and 800 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1 538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TAIOO, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37± 2 °C for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.
Results	
• **Remarks**	C6-C8 branched alkyl acetate ester, did not induce significant increases in revertant colonies (≥ 3 times the vehicle controls) in any of the tested

strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains.

Toxicity was observed in the initial assay in the following dose levels and strains: at 100 µg/plate TA1537 (+S9), ≥ 200 µg/plate in TA100 (-S9), TA1535 (+S9), TA1537 (-S9), TA1538 (±S9); ≥ 400 µg/plate in TA98 (±S9), TA1535 (-S9), TA1537 (+S9), and ≥ 600 µg/plate in TA100 (+S9). In the repeat assay, toxicity was observed at doses ≥ 400 µg/plate in TA100 (-S9) and TA1537 (-S9), and at 600 µg/plate in TA98 (-S9), TA1535 (-S9), TA1537 (+S9), and TA1538 (±S9). The nontreated and vehicle controls responded in a manner consistent with data from previous assays.

- **Conclusion** — C6-C8 branched alkyl acetate ester was not mutagenic in any strain of Salmonella typhimurium tested, even at doses that produced evidence of toxicity.

Data Quality — 1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference — Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Assay with C6-C8 Branched Alkyl Acetate Ester. Project # 164025.

Genetic Tox *In Vitro*

Test Substance	C6-C8 branched alkyl acetate ester
CAS #	90438-79-2
Method	Galloway, et al, Development of a standard *protocol* for *in* vitro *cytogenetic testing with Chinese hamster ovary cells: comparison of results* for 22 *compounds in* two *laboratories.* Environ, Mutagen. 7:1-51, 1985.
Type	In Vitro Chromosomal Aberration Assay in CHO Cells
System of Testing	Cultured Chinese hamster ovary (CHO) cells
GLP	Yes
Year	1997
Remarks for Test Conditions	Treatment group doses (11 total in initial and repeat assays) ranged from 80-240 µg/mL in the 20-hour initial test; 40-200 µg/mL in the 20- and 44-hour repeat assays. S9 activation was used in doses ranging from 80-240 µg/mL in the 20-hour initial assay and ranging from 40-200 µg/mL in the 20- and 44-hour repeat assays. Vehicle in all assays was DMSO (not exceeding 1 .O% final volume to ensure normal cell viability and growth rate). Positive controls, N-methyl-N-Nitro-N-Nitrosoguanidine (MNNG - clastogen that does not require metabolic activation) and 7,12-Dimethylbenz[a]anthracene (DMBA- clastogen that requires metabolic activation) were used as positive controls in the nonactivated series and activated series, respectively.
Results	C6-C8 branched alkyl acetate ester, was tested in a 20-hour chromosome aberration assay using Chinese hamster ovary cells with and without metabolic activation. A repeat assay was also performed using 20-hour and 44-hour harvests. For the initial 20-hour harvest data, there was a notable decrease in the percent cell confluency at concentrations ≥ 180 µg/mL with activation and at concentrations ≥ 140 µg/mL without activation. Cell morphology and mitotic indices were acceptable at or below these levels and cell death was prevalent above these levels. For the repeat assay, there were no statistically significant dose-related trends in the percentage of aberrant cells and none of the test concentrations were statistically different than the vehicle control in the 20 or 44 hour activated or nonactivated series. The percentage of aberrant cells in the vehicle control groups ranged from 1% to 2.0%, and the percentage of aberrant cells in the treated groups ranged from 0.0% to 2.6% for the 20 and 44 hour activated and nonactivated series.
Remarks	All negative and positive controls used in this study performed in an appropriate manner.
Conclusion	C6-C8 branched alkyl acetate ester was considered negative for inducing chromosome aberrations under the conditions of this test at doses up to 180 µg/mL with and 140 µg/mL without metabolic activation.

Data Quality

1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Exxon Biomedical Sciences, inc., East Millstone, NJ, USA, In Vitro Chromosomal Aberration Assay in CHO Cells with C6-C8 Branched Alkyl Acetate Ester. Project # 164032.

Acute Dermal Toxicity

Test Substance	C7-C9 branched alkyl acetate ester
CAS #	108419-32-5
Method	Experimental (Non-regulatory)
Type	Limit
GLP	Compliant
Year	1983
Species/Strain	Rabbit (New Zealand White)
Sex	Male & Female
#/sex/dose	3
Vehicle	None
Route of Admin	Dermal Application
Doses	3160 mg/kg
• **Doses/time**	Single application / 24-Hour Occlusive Patch
• **Post Dose Observation Period**	14 Days

Results

• **LD50**	>3.16 glkg
• **Remarks**	Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14. One animal was sacrificed on Day 11 due to severe weight loss. The surviving five animals showed slight weight gain through the study. Dermal evaluations ranged from no erythema to moderate to severe. Edema scores ranged from no edema to slight edema. Desquamation was noted in four animals during the study. The animal terminated on Day 11 revealed kidney discoloration, small spleen, cecum and ileum, and brown material in the stomach. The remaining five animals showed no abnormalities at necropsy.
• **Conclusion**	C7-C9 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Data Quality	1 - Reliable without Restrictions, No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Bio/dynamics Inc., East Millstone, NJ, USA, Acute Dermal Toxicity Study in the Rabbit with C7-C9 Branched Alkyl Acetate Ester. Project # 330306.

Genetic Tox *In Vitro*

Test Substance	C7-C9 branched alkyl acetate ester
CAS #	108419-32-5
Method	FIFRA 84-2
Type	Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)
System of Testing	Bacterial
GLP	Yes
Year	1994
Species/Strain	S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538
Metabolic Activation	
• **Species/cell type**	Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9)
Concentrations Tested	25, 50, 100, 200, 400, and 600 µg/plate (__ repeat assay only; ___ initial assay only)
Vehicle	DMSO
Remarks for Test Conditions	There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 25, 50, 100, 200,400, or 600 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37 ± 2 °C for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.

Results

- **Remarks**

C7-C9 branched alkyl acetate ester, did not induce significant increases in revertant colonies (≥ 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains.

In the initial and repeat assay, neither a positive response nor a dose related increase was observed for any of the tester strains. Toxicity, either a reduction in the number of revertant colonies or a reduction in the background lawn, was observed for all five tester strains with an without metabolic activation in both the initial and repeat assays, except for tester strain TA1535 with metabolic activation for the repeat assay. The nontreated and vehicle controls responded in a manner consistent with data from previous assays.

- **Conclusion**

C7-C9 branched alkyl acetate ester was not mutagenic in any strain of Salmonella typhimurium tested.

Data Quality

1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay with C7-C9 Branched Alkyl Acetate Ester. Project # 168825.

Genetic Tox *In Vivo*

Test Substance	C7-C9 branched alkyl acetate ester
CAS #	108419-32-5
Method	TSCA 798.5395
Type	In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method
GLP	Yes
Year	1994
Species	Mouse
Strain	Crl:CD-1 (VAF/Plus)
Sex	Males and Females
Number	5/sex/dose
Route of Administration	Oral Gavage
Doses/time	0.825, 1.25, and 2.5 grams/kg / Single dose
Test Period	24, 48 and 72 hours
Vehicle	Corn Oil
Positive Control	Cyclophosphamide (40 mg/kg) in reagent grade water by oral gavage
Remarks	The test substance and the vehicle were administered as a single dose by oral gavage. The vehicle was dosed at a volume equal to the test substance volume. The positive control was administered as a single dose at a volume equal to the test substance volume. Animals from the appropriate groups were sacrificed at approximately 24, 48, and 72 hours. Animals dosed with Cyclophosphamide were sacrificed at 24 hours only. Immediately following sacrifice, both femurs from each animal were removed and the bone marrow was aspirated, flushed in fetal bovine serum and centrifuged. The cell pellet was resuspended and two slide smears/animal were made. The slides were stained with Acridine Orange and wet mounted. Slides were then evaluated for presence of micronuclei (1000 polychromatic erythrocytes/animal were evaluated).
Results	A statistically significant increase in the mean number of micronucleated polychromatic erythrocytes was not seen at any dose level. Cytotoxicity, shown by a dose-related decrease in the percentage of polychromatic erythrocytes, was observed for both sexes at the 48-hour sampling time (regression coefficient $p<0.01$). The two highest dose groups were statistically different from the vehicle control. Both the positive

(cyclophosphamide) and negative (vehicle carrier) controls responded in an appropriate manner.

Remarks The test material is considered to be toxic to bone marrow in CD-1 mice under the conditions of this test based on the decrease in the mean percent of polychromatic erythrocytes at the 48-hour sampling time.

Conclusion C7-C9 branched alkyl acetate ester did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-l mice. Therefore, it is not considered mutagenic under the conditions of this assay.

Data Quality 1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method with C7-C9 Branched Alkyl Acetate Ester. Project # 168830.

Repeated Dose Oral Toxicity

Test Substance	C7-C9 branched alkyl acetate ester
CAS #	108419-32-5
Method	EPA TSCA 798.2650
Type	13-Week Repeated Dose Oral Toxicity
GLP	Yes
Year	1985
Species/Strain	Rat - Sprague-Dawley
Sex	Male & Female
#/sex/dose	20
Vehicle	None
Route of Admin	Gavage
Duration of Test	90-Day
Doses	0, 0.1, 0.5, and 1 .O g/kg/day
• **Volume**	< 1 .1 11 ml/kg (controls received a dose of water volumetrically comparable to the dosage administered to the high dose group, 1 .1 11 ml/kg)
• **Remarks**	Clinical laboratory studies (hematology and serum chemistry) were performed pretest on 5 males and 5 females (non-study animals), on 5 animals/sex/dose after 45 days (interim sacrifice), and all animals at study termination. Blood samples were collected from the abdominal aortas following an overnight fast. At 45 days, a complete necropsy was performed and livers were collected, weighed and preserved. After 13 weeks, all surviving animals were weighed, anesthetized and sacrificed by exsanguination. Complete necropsies were performed.

Results

. **NOAEL**	1 .O g/kg/day
• **Remarks**	Liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and do not indicate toxic effects. Microscopic evaluation of the kidneys revealed evidence of mild tubular nephropathy only in the high-dose male rats that were consistent with alpha-2u-globulin effects.
• **Conclusion**	Oral administration of C7-C9 branched alkyl acetate ester daily, 5 days/week for 13 weeks, to rats produced minimal signs of systemic toxicity. There was no treatment-related mortality. The in-life clinical

observations were primarily oral and dermal irritation (no clear dose-response). Weekly mean body weights and food consumption values were not significantly altered compared to controls. The qualitative hematologic data were unremarkable at all dose levels for the interim and terminal evaluations. At the terminal sacrifice, there were no biologically significant differences between treated and control animals for the measured clinical chemistries. Terminal liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and not indicative of toxic effects. All other organ weights were comparable to control values. Microscopic evaluation of the kidneys showed evidence of mild tubular nephropathy only in the high-dose male rats that were consistent with alpha-2u-globulin effects. Histopathology review of all other tissues from high-dose animals, including reproductive organs (testes, epididymides, prostate, seminal vesicles, ovaries, uterine horns, cervix, and corpus of the uterus, and vagina), showed normal morphology. The lowest observable effect level was 500 mg/kg. No effects were observed at 100 mg/kg.

Data Quality

1 - Reliable without Restrictions. No circumstances occurred that affected the quality or integrity of the data.

Reference

Bio/dynamics Inc., East Millstone, NJ, USA, Subchronic Oral Gavage Study in Rats; Project # 230370.

Developmental Toxicity / Teratogenicity

Test Substance	C7-C9 branched alkyl acetate ester
CAS #	108419-32-5
Method	**EPA 798.4900** Guideline
Type	Developmental Toxicity
GLP	Yes
Year	1985
Species	Rat
Strain	Sprague-Dawley
Route of Admin	Oral Gavage
Doses/Concentration	**0,** 100, 500 and 1000 mg/kg
Sex	Female
Exposure Period	Gravid Day 6-15
Frequency of Treatment	Single Dose Daily
Control Group	Sham-Treated with distilled water at 1000 mg/kg
Duration of Test	Gravid Day 20
Statistical Methods	Maternal body weight, body weight change, food consumption, uterine data (i.e., corpora lutea, implants, resorptions), and malformation data were analyzed with Bartlett's test of homogeneity of variance to determine if groups had equivalent variances at the 15 level of significance. If not significantly different, groups were compared using a one-way standard analysis of variance (ANOVA). If significant differences among means were detected, Duncan's test was used to determine the treated group that differed from control. Fetal weights and crown-rump lengths were analyzed using individual fetal values by a standard nested analysis of variance with values nested within dams and dams nested within groups. If differences within groups were indicated, the least-significant-difference technique was used to determine the group(s) that differed from control. If the groups did not have equivalent variances at the 1% level, then a Kruskal-Wallis test (nonparametric) was used to assess differences in group means. If the means were different, a rank sum comparison was used to determine the treatment group that differed from control.
#/sex/dose	22 Mated Females
Vehicle	None

Results

- **Maternal NOEL** 100 mglkglday
- **Maternal NOAEL** 500 mglkglday
- **Pup NOEL** 500 mglkglday
- **Pup NOAEL** 500 mg/kg/day
- **Remarks** For the 1000 mg/kg group, there was a slightly increased incidence of malformations, although the different types of malformations, observed did not suggest a characteristic pattern of anomalies. No developmental toxicity was observed at the maternally toxic dose of 500 mg/kg or the maternally nontoxic dose of 100 mg/kg.
- **Conclusion** C7-C9 branched alkyl acetate ester, was administered at 0, 100, 500, and 1000 mg/kg on gestation days 6-l 5 in a developmental toxicity study in rats. Maternal toxicity was seen at the 500 and 1000 mg/kg doses as evidenced by decreases in body weight and food consumption. There was a slight increase in fetal malformations and embryotoxicity in the 1000 mg/kg group only; no adverse fetal effects were observed in the 100 and 500 mg/kg groups.

Data Quality 1 - Reliable without Restrictions. No circumstances occurred that affected the quality or integrity of the data.

Reference Bio/Dynamics Inc., East Millstone, NJ, USA, Oral Teratology Study in Rats Project # 330334.

Acute Dermal Toxicity

Test Substance	C8-C10 branched alkyl acetate ester
CAS #	108419-33-6
Method	Experimental (Non-regulatory)
Type	Limit
GLP	Compliant
Year	1983
Species/Strain	Rabbit (New Zealand White)
Sex	Male & Female
#/sex/dose	3
Vehicle	None
Route of Admin	Dermal Application
Doses	3160 mg/kg
• **Doses/time**	Single application / 24-Hour Occlusive Patch
• **Post Dose Observation Period**	14 Days

Results

. **LD50**	>3.16 g/kg
• **Remarks**	Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14. Erythema was noted in all animals at 24 hours and continued in four animals through Day 14. Edema was seen in three animals at 24 hours. No animals showed edema by the Day 7 evaluation. Desquamation was seen in one animal on Day 7, three animals on Day 10 and remained in two animals at the Day 14 termination. One male and two females at Day 7 and one male and one female showed slight decreases in body weight. Food consumption was reduced on Day 1 only. Postmortem examination revealed gallbladder and salivary gland abnormalities, kidney discoloration, a urinary bladder abnormality, hair in two stomachs and ano-genital staining.
• **Conclusion**	C8-C10 branched alkyl acetate ester has a low order of percutaneous toxicity when administered in a single dose to intact rabbit skin at 3.16 g/kg.

Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Bio/dynamics inc., East Millstone, NJ, USA, Acute Dermal Toxicity Study in the Rabbit with C8-C10 Branched Alkyl Acetate Ester. Project # 330406.

Acute Dermal Toxicity

Test Substance	C9-C11 branched alkyl acetate ester
CAS #	108419-34-7
Method	Experimental (Non-regulatory)
Type	Limit
GLP	Compliant
Year	1984
Species/Strain	Rabbit (New Zealand White)
Sex	Male & Female
#/sex/dose	3
Vehicle	None
Route of Admin	Dermal Application
Doses	3160 mg/kg
• **Doses/time**	Single application / 24-Hour Occlusive Patch
• **Post Dose Observation Period**	14 Days
Results	
. **LD50**	>3.16 glkg
• **Remarks**	Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14. There were no deaths during the course of this study. Three of six animals gained weight during the study. Clinical in-life observations included ano-genital staining, ocular discharge, unthrifty coat, nasal discharge and poor food consumption. Erythema and edema were slight to well defined. Desquamation was also observed. Postmortem examination revealed kidney discoloration, an encapsulated salivary gland, an enlarged cervical lymph node and hair present in the stomach.
• **Conclusion**	C9-C11 branched alkyl acetate ester has a low order of percutaneous toxicity when administered in a single dose to intact rabbit skin at 3.16 g/kg.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference

Bio/dynamics Inc., East Millstone, NJ, USA, Acute Dermal Toxicity Study in the Rabbit with C9-C11 Branched Alkyl Acetate Ester. Project # 330506.

Acute Oral Toxicity

Test Substance	Cl l-Cl4 branched alkyl acetate ester
CAS #	108419-35-8
Method	Experimental
Type	Limit
GLP	Compliant
Year	1983
Species/Strain	Rat (Sprague-Dawley)
Sex	Male & Female
#/sex/dose	5
Vehicle	None
Route of Admin	Oral Gavage
Doses	
• **Doses/time**	Single (18 Hr Fasted)
• **Vol. Admin.**	5.721 ml/kg (1 .1 - 1.9 ml)
• **Post Dose Observation Period**	14 Days
Results	
. **LD50**	>5 g/kg
• **Remarks**	There were no deaths during this study. Nine of 10 animals showed staining in the ano-genital area on Days 1 and 2, and for 1 animal on Day 3. Soft stool was noted for 1 animal at 6 Hrs PD and white gelatinous material on the penis was noted for 1 animal on Day 1. There were no observable abnormalities noted after the Day 3 observations. All animals except one showed an increase over pre-dose weights except one animal that appeared to have had an incorrect pre-dose weight recorded. Six of 10 animals showed no observable abnormalities during postmortem examination. Four animals showed lung discoloration typical of findings resulting from carbon dioxide asphyxiation.
• **Conclusion**	Cl 1 -Cl4 branched alkyl acetate ester elicited minimal signs of acute systemic toxicity when administered orally. Signs of slight toxicity (staining of the fur and soft stool) were limited to the first 3 days.

Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Bio/dynamics, East Millstone, NJ, USA, Acute Oral Toxicity Studv in the Rat; Project # 330601.

Acute Dermal Toxicity

Test Substance	Cl 1 -C14 branched alkyl acetate ester
CAS #	108419-35-8
Method	Experimental (Non-regulatory)
Type	Limit
GLP	Compliant
Year	1984
Species/Strain	Rabbit (New Zealand White)
Sex	Male & Female
#/sex/dose	3
Vehicle	None
Route of Admin	Dermal Application
Doses	3160 mg/kg
• **Doses/time**	Single application / 24-Hour Occlusive Patch
• **Post Dose Observation Period**	14 Days
Results	
. **LD50**	>3.16 g/kg
• **Remarks**	There were no overt signs of systemic toxicity. Five of 6 rabbits showed slight body weight decreases at Day 7; only 2 animals continued to have decreased body weight at 14 days. Slight dermal irritation persisted in 4 of 6 test animals through termination of the study. In general, dermal responses were considered minimal and transient in nature. At post mortem examination, 3 of 6 animals showed no observable abnormalities. Liver and salivary gland discoloration was observed in one animal; kidney discoloration and spleen enlargement in another; and alopecia in the third animal.
• **Conclusion**	Cl l-Cl4 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Bio/dynamics Inc., East Millstone, NJ, USA, Acute Dermal Toxicity Study in the Rabbit; Project # 330606.

Genetic Tox *In Vitro*

Test Substance	Cl l-Cl4 branched alkyl acetate ester
CAS #	**108419-35-8**
Method	FIFRA 84-2
Type	Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)
System of Testing	Bacterial
GLP	**Yes**
Year	**1994**
Species/Strain	S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538
Metabolic Activation	
• Species/cell type	Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9)
Concentrations Tested	156, 312.5, 625, 1250, 2500, 5000, and 10000 µg/plate (__ repeat assay only; __ initial assay only)
Vehicle	DMSO
Remarks for Test Conditions	There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 156, 312.5, 625, 1250, 2500, 5000, and 10000 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37 ± 2 °C for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.

Results

• **Remarks**	Cl l-Cl4 branched alkyl acetate ester, did not induce significant increases in revertant colonies (≥ 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains. In the initial and repeat assay, neither a positive response nor a dose related increase was observed for any of the tester strains. Toxicity, either a reduction in the number of revertant colonies or a reduction in the background lawn, was not observed. Test substance beading was observed for all tester strains, both with and without metabolic activation at 1250 through 10000 μg/plate. The nontreated and vehicle controls responded in a manner consistent with data from previous assays.
• **Conclusion**	Cl l-Cl4 branched alkyl acetate ester was not mutagenic in any strain of Salmonella typhimurium tested and was not toxic in any strain tested under the conditions of this study.
Data Quality	1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.
Reference	Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay; Project # 168925.

Genetic Tox *In Vivo*

Test Substance	Cl I -C14 branched alkyl acetate ester
CAS #	108419-35-8
Method	TSCA 798.5395
Type	In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method
GLP	Yes
Year	1994
Species	Mouse
Strain	Crl:CD-1 (VAF/Plus)
Sex	Males and Females
Number	5/sex/dose
Route of Administration	Oral Gavage
Doses/time	0.45, 0.90, and I .80 grams/kg / Single dose
Test Period	24, 48 and 72 hours
Vehicle	Corn Oil
Positive Control	Cyclophosphamide (40 mg/kg) in reagent grade water by oral gavage
Remarks	The test substance and the vehicle were administered as a single dose by oral gavage. The vehicle was dosed at a volume equal to the test substance volume. The positive control was administered as a single dose at a volume equal to the test substance volume. Animals from the appropriate groups were sacrificed at approximately 24, 48, and 72 hours, Animals dosed with Cyclophosphamide were sacrificed at 24 hours only. Immediately following sacrifice, both femurs from each animal were removed and the bone marrow was aspirated, flushed in fetal bovine serum and centrifuged. The cell pellet was resuspended and two slide smears/animal were made. The slides were stained with Acridine Orange and wet mounted. Slides were then evaluated for presence of micronuclei (I 000 polychromatic erythrocytes/animal were evaluated).
Results	A dose-related decrease in the percentage of polychromatic erythrocytes was observed for the female 48-hour sampling time (regression coefficient $p<0.01$). However, none of the dose groups were statistically different from the control. The positive control (40 mg/kg cyclophosphamide) induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes ($p<0.01$)

which indicates that the positive control is clastogenic and is responding in an appropriate manner. Vehicle carrier control values for the mean percent of polychromatic erythrocytes and for the mean percent of micronucleated polychromatic erythrocytes responded in an appropriate manner.

Remarks The test material is considered to be toxic to bone marrow in CD-1 mice based on the decrease in the mean percent of polychromatic erythrocytes at the 48-hour sampling time.

Conclusion Cl l-Cl4 branched alkyl acetate ester did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-l mice. Therefore, it is not considered mutagenic under the conditions of this assay.

Data Quality 1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

Reference Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method, Project # 168930

Repeated Dose Oral Toxicity

Test Substance	Cl 1 -C14 branched alkyl acetate ester
CAS #	108419-35-8
Method	EPA TSCA 798.2650
Type	13-Week Repeated Dose Oral Toxicity
GLP	Yes
Year	1985
Species/Strain	Rat - Sprague-Dawley
Sex	Male & Female
#/sex/dose	20
Vehicle	None
Route of Admin	Gavage
Duration of Test	90-Day
Doses	0, 0.1, 0.5, and 1 .O g/kg/day
• **Volume**	≤ 1 ,111 ml/kg (controls received a dose of water volumetrically comparable to the dosage administered to the high dose group, 1 .l 11 ml/kg)
• **Remarks**	Clinical laboratory studies (hematology and serum chemistry) were performed pretest on 5 males and 5 females (non-study animals), on 5 animals/sex/dose after 45 days (interim sacrifice), and all animals at study termination. Blood samples were collected from the abdominal aortas following an overnight fast. At 45 days, a complete necropsy was performed and livers were collected, weighed and preserved. After 13 weeks, all surviving animals were weighed, anesthetized and sacrificed by exsanguination. Complete necropsies were performed.
Results	
. **NOAEL**	1 .O glkglday
• **Remarks**	Liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and do not indicate toxic effects. Microscopic evaluation of the kidneys revealed evidence of mild tubular nephropathy only in the high-dose male rats that were consistent with alpha-2u-globulin effects.
• **Conclusion**	Oral administration of Cl 1 -Cl 4 branched alkyl acetate ester daily, 5 days/week for 13 weeks, to rats produced minimal signs of systemic toxicity. There was no treatment-related mortality. The in-life clinical

observations were primarily oral and dermal irritation (no clear dose-response). Weekly mean body weights and food consumption values were not significantly altered compared to controls. The qualitative hematologic data were unremarkable at all dose levels. At the terminal sacrifice, glucose values for the 0.5, and 1 .O g/kg/day males were lower than controls and the total protein values for the 1 .O g/kg/day females were higher than controls. Terminal liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and not indicative of toxic effects. Microscopic evaluation of the kidneys showed evidence of mild tubular nephropathy in the mid- and high-dose male rats that were consistent with alpha-2u-globulin effects. Histopathology review of all other tissues from high-dose animals, including reproductive organs (testes, epididymides, prostate, seminal vesicles, ovaries, uterine horns, cervix/corpus of the uterus, and vagina), showed normal morphology. The lowest observable effect level was 500 mg/kg. No effects were observed at 100 mg/kg.

Data Quality

1 - Reliable without Restrictions. No circumstances occurred that affected the quality or integrity of the data.

Reference

Bio/dynamics Inc., East Millstone, NJ, USA, Subchronic Oral Gavage. Study in Rats; Project # 252170.

Developmental Toxicity / Teratogenicity

Test Substance	Cl l-Cl4 branched alkyl acetate ester
CAS #	108419-35-8
Method	EPA 798.4900 Guideline
Type	Developmental
GLP	Yes
Year	1985
Species	Rat
Strain	Sprague-Dawley
Route of Admin	Oral Gavage
Doses/Concentration	0, 500, 1300, and 2500 mg/kg
Sex	Female
Exposure Period	Gravid Day 6-l 5
Frequency of Treatment	Single Dose Daily
Control Group	Sham-Treated with distilled water at 2.5 g/kg
Duration of Test	Gravid Day 20
Statistical Methods	Maternal body weight, body weight change, food consumption, uterine data (i.e., corpora lutea, implants, resorptions), and malformation data were analyzed with Bartlett's test of homogeneity of variance to determine if groups had equivalent variances at the 15 level of significance. If not significantly different, groups were compared using a one-way standard analysis of variance (ANOVA). If significant differences among means were detected, Duncan's test was used to determine the treated group that differed from control. Fetal weights and crown-rump lengths were analyzed using individual fetal values by a standard nested analysis of variance with values nested within dams and dams nested within groups. If differences within groups were indicated, the least-significant-difference technique was used to determine the group(s) that differed from control. If the groups did not have equivalent variances at the 1% level, then a Kruskal-Wallis test (nonparametric) was used to assess differences in group means. If the means were different, a rank sum comparison was used to determine the treatment group that differed from control.
#/sex/dose	22 Mated Females
Vehicle	None

Results

- **Maternal NOEL** 500 mg/kg/day
- **Maternal NOAEL** 500 mg/kg/day
- **Pup NOEL** 2500 mg/kg/day
- **Pup NOAEL** 2500 mg/kg/day

Remarks There were no statistically significant deleterious effects on survival, fetal body weight, crown-rump length or malformations at any dose.

Conclusion Cl l-Cl4 branched alkyl acetate ester was administered at 0, 500, 1300, and 2500 mg/kg on gestation days 6-1 5 in a developmental toxicity study in rats. Maternal toxicity was seen at the 1300 and 2500 mg/kg doses as evidenced by decreases in body weight. There were no statistically significant deleterious effects on fetal survival, body weight, or crown-rump length and no evidence of treatment-related malformations.

Data Quality 1 - Reliable without Restrictions. No circumstances occurred that affected the quality or integrity of the data.

Reference Bio/dynamics Inc., East Millstone, NJ, USA, Oral Teratology Study in Rats; Project # 352134.

Fish Acute Toxicity

Test Substance:	CAS No. 88230-35-7, C6 branched and linear alkyl acetate ester
Method/Guideline:	OECD 203
Year (guideline):	1992
Type (test type):	Semi-Static Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1995
Species:	Rainbow Trout (Oncorhynchus mykiss)
Analytical Monitoring:	Yes (TOC)
Exposure Period:	96 hour
Statistical Method:	Trimmed Spearman Karber Method
Test Conditions: - Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	Individual test concentrations were prepared by adding the test substance to 17L of laboratory blend water in 20L glass carboys. The solutions were mixed for 24 hours at test temp (13-17 Deg C) with a vortex of <1 0%. Mixing was performed using a magnetic stir plate and teflon stir bar (132 rpm). After mixing, the solutions were allowed to settle for one hour and the Water Accommodated Fraction (WAF) was removed via a glass tube from the bottom of vessel. Test vessels were 4.0L aspirator bottles containing 4.5L of solution (no headspace). Test vessels were sealed with foil covered stoppers. Three replicates of each concentration were tested, each containing 5 fish. Approximately 80% of each solution was renewed daily from a freshly prepared WAF. Nominal treatment levels were control, 0.5, 1.3, 3.2, 8.0, and 20.0mg/L Test temperature was 15.2 Deg C. Lighting was 62 to 69 ft. candles with gradual 16 hrs light and 8 hrs dark. Dissolved oxygen was 9.0 to 9.4mg/L for "new" solutions and 6.3 to 8.5mg/L for "old" solutions. The pH ranged from 7.4 to 7.7 for "new" solutions and 7.0 to 7.4 for "old" solutions. Fish supplied by Thomas Fish Co.; age = approximately 6 weeks; mean wt.=0.333g; mean total length=3.6cm; test loading=0.37g of fish/L.

Results:

Units/Value:

96 hour LL50 = 11 .9mg/L (95% CI 10.6 to 13.4) based upon nominal values.

Results con't

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Analytical method used was Total Organic carbon (TOC). The fish were slightly smaller than the guideline suggestion of 4.0 to 6.0cm, which were purposely selected to help maintain oxygen levels in the closed system.

Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)
Control	0
0.5	0
1.3	0
3.2	0
8.0	1
20.0	15

*1 5 fish added at test initiation

Conclusion:

Reliability: (1) Reliable without restriction

Reference: Exxon Biomedical Sciences Inc. 1995. Acute Fish Toxicity Test with Rainbow Trout. Study #101558.

Other (source): ExxonMobil Chemicals

Invertebrate Acute Toxicity

Test Substance:	CAS No. 88230-35-7; C6 branched and linear alkyl acetate ester
Method/Guideline:	OECD 202
Year (guideline)	1992
Type (test type):	Static Acute Daphnid Toxicity Test
GLP:	Yes
Year (study performed):	1995
Species:	Water Flea (Daphnia magna)
Analytical Monitoring:	Yes (TOC)
Exposure Period:	48 hour
Statistical Method:	Finney, D.J. probit procedure of SAS
Test Conditions: • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**	Individual treatment solutions were prepared as water accommodated fractions (WAFs). A WAF was prepared by adding test substance to 1.8L of solution in a 2.0 liter aspirator bottle and mixing with a magnetic stir plate and bar. Mixing vortex was <10%. After mixing for 24 hours at room temperature, the WAF was allowed to settle for one hour and removed from the port at the bottom of the bottle. Test vessels were 125ml glass beakers filled with 140ml of solution and covered. Four replicates were prepared for each treatment. Each replicate contained 5 organisms. Nominal treatment levels were: control, 0.1, 0.5, 1 .0, 5.0, and 1 O.Omg/L Test temperature was 20.7 Deg C. Lighting was 58 to 59 ft candles with 16 hrs light and 8 hrs dark. Dissolved oxygen was 7.3 to 8.8mg/L. The pH ranged from 7.3 to 8.3. Organisms were supplied by in-house cultures; age = <24 hours old. Parents age = 14 to 18 days old.

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

48 hour LL50 = 7.6mg/L (95% Cl 5.9 to 10.7mg/L) based upon nominal values.

Analytical method used was Total Organic Carbon **(TOC).**

Nominal Conc. (mg/L)	Daphnia Total Mortality (@48 hrs)
Control	1
0.1	2
0.5	1
1.0	3
5.0	5
10.0	14

*20 Daphids total added at test initiation.
Mortality is defined as immobilized.

Conclusion:

Reliability: (1) Reliable without restriction

Reference: Exxon Biomedical Sciences, Inc. 1995. Acute Daphnid Toxicity Test. Study #1 01542B.

Other (source): ExxonMobil Chemicals

Algal Toxicity

Test Substance:	CAS No. 88230-35-7, C6 branched and linear alkyl acetate ester
Method/Guideline:	OECD 201, Annex V
Year (guideline):	**1992**
Type (test type):	Algal Toxicity Test
GLP:	**Yes**
Year (study performed):	**1995**
Species/Strain:	Fresh-Water Green Algae (Selenastrum capricornutum)
Analytical Monitoring:	**Yes**
Exposure Period:	96 hour
Statistical Method:	Proc regression procedure of SAS, Anova procedure of SAS for NOEC
Test Conditions: • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organism culture, age.**	Individual test treatment solutions were prepared as Water Accommodated Fractions (WAFs). Test material was added to 1.8L of algal media in 2.0L aspirator bottles. The mixing vessels were sealed with foil covered stoppers and mixed on magnetic stir plates with teflon coated stir bars for 24 hours at room temperature. After mixing the solutions were allowed to settle for one hour and the WAF was removed from the bottom of the mixing vessel via the port and used for testing. Test vessels were 125ml glass Erlenmeyer flasks that were completely filled (140ml) with treatment solution and inoculated with algae. Samples were taken daily for cell counts. Four replicates were prepared for each treatment level. The initial algal concentration was 1 .O x 1 0^4 cells/ml. All test replicates were placed on a shaker table at 100 oscillations per minute during the study. To facilitate mixing, with no headspace, 10 glass beads were placed in each vessel. Biomass was calculated as the area under the growth curve. Nominal treatment levels were 8.0, 31 .0, 62, 125, and 250mg/L Test temperature was 23.6 Deg. C. Lighting was continuous at 4300 to 4663 Lux. The pH was 7.5 at test initiation and ranged from 8.3 to 10.4 at test termination.
Results: **Units/Value:** **Measurement (cells/growth)**	96 hour EL50b=40.1 mg/L (biomass) 96 hour EL50gr=32.1 mg/L (growth rate) 72 & 96 hour NOELRb=31 .Omg/L (biomass) 72 & 96 hour NOELRgr=8.0mg/L (growth rate) Analytical method used was Dissolved Organic Carbon (DOC). No excursions from the protocol were noted.

Results con't

Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.

Nominal Conc. mg/L	Growth - 72 & 96 hr (% Inhibition)		Mean Cell Conc. - 96 hr (cells/ml)
Control	n/a	n/a	8.8 x 10^5
8.0	1.2	-4.2*	1.1 x 10^6
31 .0	8.4	-3.5*	1.1 x 10^6
62.0	80.2	84.4	2.6 x 10^4
125.0	94.5	97.2	9.6 x 10^3
250.0	99.9	100	3.4 x 10^3

n/a - Not applicable
● Stimulatory response

Conclusion:

Reliability: (1) Reliable without restriction

Reference: Exxon Biomedical Sciences Inc. 1995. Algal Inhibition Test. Study #101567.

Other (source): ExxonMobil Chemicals

Biodegradation

Test Substance:	CAS No. 88230-35-7; C6 branched and linear alkyl acetate ester
Method/Guideline:	USEPA TSCA 40 CFR 796.3100
Year (guideline)	1988
Type (test type):	Aerobic Aquatic Biodegradation (Gledhill Shake Flask Test)
GLP:	Yes
Year (study performed):	1994
Inoculum:	Domestic activated sludge, raw sewage and soil
Exposure Period:	28 days
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Non acclimated activated sludge, sewage, soil, and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride). Test vessels were 2L Gledhill flasks located in the dark in an environmental chamber. Each test vessel was monitored for carbon dioxide via charcoal tube and air purging. Sampling was performed on Days 2, 3, 5, 7, 13, 19, and 28. Test material and positive control were tested in triplicate. Test material concentration was 30mg carbon/L. Aniline (positive control) concentration was 20 mg carbon/L. Test temperature was 19 to 23 Deg C.
Results: **Units/Value:** · **Note: Deviations from protocol or guideline, analytical method.**	Test material was readily biodegradable. Half-life was <=2 weeks. By day 28, 76.9% degradation of the test material was observed. 10% biodegradation was achieved on approximately day 2, 50% biodegradation on approximately day 13. By day 7, >60% biodegradation of positive control was observed. No excursions from the protocol were noted. Biodegradation was based on theoretical Carbon Dioxide values and the cumulative Carbon Dioxide produced by the test substances.

Sample	% Degradation* 28)y	Mean % Degradation (day 28)
Test Substance	74.6, 82.0, 74.1	76.9
Aniline	86.5, 83.7, 83.9	84.7

* replicate data

Conclusion:

Reliability: (1) Reliable without restriction

Reference: Exxon Biomedical Sciences Inc. 1994. Aerobic Aquatic Biodegradation, Gledhill Shake Flask Test. Study #168687.

Other (source): ExxonMobil Chemicals

Stability in Water

Test Substance:	CAS No. 88230-35-7; C6 branched and linear alkyl acetate ester
Method/Guideline:	OECD Guideline 111 and EC Annex V Guideline C.7
Year (guideline):	1992
Type (test type):	Hydrolysis (abiotic)
GLP:	Yes
Year (study performed):	1995
Exposure Period:	27- 45 days (definitive test)
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The hydrolysis of the test substance was evaluated at 3 relevant pH values. A preliminary test of 95ug/ml at pH values of 4, 7, and 9 showed stability at pH 4 and 7. A definitive test was performed at 98 ug/ml and a pH value of 9 at varying temperatures (15 and 25 Deg C). A sufficient volume of test substance stock solution was added to a buffer solution to yield a nominal concentration of 98 ug/ml (less than half of expected maximum water solubility concentration). Test samples were stored in the dark in laboratory incubators and the temperature recorded daily. Test vessels were sterilized VOA vials containing a buffer solution with the test substance and no headspace. Test substance concentrations were measured by GC-FID.
Results: **Units/Value:**	Half life at pH 9 and 25 Deg C = 13 days. Half life at pH 9 and 15 Deg C = 36 days.
• **Note: Deviations from protocol or guideline, analytical method.**	Test substance was stable at pH 4 and pH 7. Less than 5% degradation was measured over a period of 5 days at these two pH values. Hydrolysis of test substance occured at pH 9, with 35% degradation observed after day 1 and 95% after day 5.
Conclusion:	Hydrolysis of the test substance is not expected to be a significant mechanism of abiotic degradation in natural bodies of water where the temperature is generally less than 25 Deg C and the pH is at or below 7.
Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1995 Abiotic Degradation Hydrolysis as a Function of pH. Study #101 590.
Other (source):	ExxonMobil Chemicals

Fish Acute Toxicity

Test Substance:	CAS No. 90438-79-2, C6 - C8 branched alkyl acetate ester
Method/Guideline:	OECD 203
Year (guideline):	1992
Type (test type):	Semi-Static Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1997
Species:	Rainbow Trout (Oncorhynchus mykiss)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Trimmed Spearman Karber Method
Test Conditions: - Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	Individual test concentrations were prepared by adding the test substance, weighed on teflon disks, to 12 L of laboratory blend water in 13L glass aspirator bottles. The solutions were mixed for 24 hours at room temp (20-24 Deg C) with a vortex of <10% (3 cm vortex). Mixing was performed using a magnetic stir plate and teflon stir bar. After mixing, the solutions were allowed to settle for one hour and the Water Accommodated Fraction (WAF) was removed via port at the bottom of vessel. Test vessels were 4.0L aspirator bottles containing 4.0L of solution (no headspace). Test vessels were sealed with foil covered stoppers. Two replicates of each concentration were tested, each containing 5 fish. Approximately 80% of each solution was renewed daily from a freshly prepared WAF. Nominal treatment levels were control, 2.0, 4.5, 10.0, 23.0, and 50.0mg/L, which measured: 1.2, 1.49, 5.39, 21 .1, and 43.6mg/L, respectively, and are based on the mean of samples taken from the new and old solutions. Test temperature was 13.6 Deg C. Lighting was 16 hrs light and 8 hrs dark. Dissolved oxygen was 8.3 to 10.4mg/L for "new" solutions and 4.5 to 7.9mg/L for "old" solutions. The pH ranged from 7.3 to 8.4 for "new" solutions and 6.7 to 7.6 for "old" solutions. Fish supplied by Thomas Fish Co.; age = approximately 6 weeks; mean wt.=0.319g; mean total length=3.5cm; test loading=0.399g of fish/L.

Results:

Units/Value:

96 hour LC50 = 8.18mg/L (95% Cl 5.85 to 11.4) based upon measured values.

Results con't

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Analytical method used was Headspace Gas Chromatography with Flame Ionization Detection (GC-FID).
The fish were slightly smaller than the guideline suggestion of 4.0 to 6.0cm, which were purposely selected to help maintain oxygen levels in the closed system.

Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	0
1.2	0
1.49	0
5.39	2
21.1	10
43.6	10

*10 fish added at test initiation

Conclusion:

Reliability: (1) Reliable without restriction

Reference: Exxon Biomedical Sciences Inc. 1997. Acute Fish Toxicity Test with Rainbow Trout. Study #164058.

Other (source): ExxonMobil Chemicals

Biodegradation

Test Substance:	CAS No. 90438-79-2; C6 - C8 branched alkyl acetate ester
Method/Guideline:	OECD 301 F
Year (guideline):	1993
Type (test type):	Ready Biodegradability, Manometric Respirometry Test
GLP:	Yes
Year (study performed):	1998
Inoculum:	Domestic activated sludge
Exposure Period:	28 days
Test Conditions:	
. **Note: Concentration prep., vessel type, replication, test conditions.**	Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride). Test vessels were 1 L glass flasks placed in a waterbath and electronically monitored for oxygen consumption. Test material was tested in triplicate, controls and blanks were tested in duplicate. Test material concentration was 52mg/L. Sodium benzoate (positive control) concentration was 52mg/L. Test temperature was 22 +/- 1 Deg C. All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.
Results:	
Units/Value:	Test material was readily biodegradable. Half-life was <1 week. By day 28, 77% degradation of the test material was observed. 10% biodegradation was achieved on day 1, 50% biodegradation on approximately day 5. By day 14, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted. Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.
• **Note: Deviations from protocol or guideline, analytical method.**	

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	73.5, 80.4, 77.4	77.1
Na Benzoate	76.0, 78.3	77.1

* replicate data

Conclusion:

Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1998 Ready Biodegradability, Manometric Respirometry. Study #1 64094A.
Other (source):	ExxonMobil Chemicals

Stability in Water

Test Substance:	CAS No. 90438-79-2; C6 - C8 branched alkyl acetate ester
Method/Guideline:	OECD Guideline 111 and EC Annex V Guideline C.7
Year (guideline):	**1992**
Type (test type):	Hydrolysis (abiotic)
GLP:	**Yes**
Year (study performed):	**1997**
Exposure Period:	17-83 days
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The hydrolysis of the test substance was evaluated at 3 relevant pH values. A preliminary test at pH values of 4, 7, and 9 showed stability at pH 4. A definitive test was performed at pH values of 7 and 9 at varying temperatures (20 and 30 Deg C for pH 9; 40 and 50 Deg C for pH 7). A sufficient volume of test substance stock solution was added to a buffer solution to yield a nominal concentration of less than 60 uglml (less than half of expected maximum water solubility concentration). Test samples were stored in the dark in laboratory incubators and the temperature recorded daily. Test vessels were sterilized VOA vials containing a buffer solution with the test substance and no headspace. Test substance concentrations were measured by GC-FID.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Half life at 50 Deg C and pH 7 = 24.3 days Half life at 40 Deg C and pH 7 = 46.5 days Half life at 30 Deg C and pH 9 = 5.29 days Half life at 20 Deg C and pH 9 = 15.8 days Test substance was stable at pH 4. Less than 10% degradation was measured over a period of 5 days. Hydrolysis of test substance occured at pH 9, with a slower but measurable rate at pH 7.
Conclusion:	Hydrolysis of the test substance is not expected to be a significant mechanism of abiotic degradation in natural bodies of water where the temperature is generally less than 20 Deg C and the pH is at or below 7.
Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1995 Hydrolysis as a Function of pH. Study #1 64090H.
Other (source):	ExxonMobil Chemicals

Fish Acute Toxicity

Test Substance:	CAS No. 108419-32-5, C7 - C9 branched alkyl acetate ester
Method/Guideline:	USEPA 560/6-82-002 Environmental Effects Test Guideline
Year (guideline):	1982
Type (test type):	Flow-Through Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1985
Species:	Fathead Minnow (Pimephales promelas)
Analytical Monitoring:	Yes (TC)
Exposure Period:	96 hour
Statistical Method:	Probit procedure by Litchfield & Wilcoxon

Test Conditions:

- Note: **Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**

A stock water accommodated fraction (WAF) was prepared by adding 267ml of the test substance to ~40L of laboratory blend water in a glass carboy. The solution was stirred for 72 hours and the 100% WAF used for testing. The WAF was administered to the test chambers via a diluter system. The diluter system comprised of glass, stainless-steel with no plasticized materials. The diluter prepared the following test treatment levels: control, 4.4, 8.8, 17.5, 35.0, and 70.0 % WAF, which measured NA, 1.39, 2.71, 4.90, 9.91, 19.86 mg/L as Total Carbon (TC). The test chambers were glass culture dishes (150 x 75mm). Two replicates with ten fish each were tested per treatment level.
Test temperature was 20.96 +/- 0.15 Deg C. Lighting was gradual on and off with 16 hours dark and 8 hour light with an intensity of 77 to 79 ft candles.
Dilution water hardness was 159 mg/L as $CaCO_3$.
The pH ranged from 7.3 to 8.1. Dissolved Oxygen ranged from 6.7 to 8.4 mg/L.
Fish were supplied by in-house laboratory; age = 13 weeks; mean wt.=0.257g; mean total length=2.4cm; test loading=0.21 g of fish/L per 24 hour period.

Results:

96 hour LL50 = 49.5 % WAF (95% CI 46.26 to 52.97) based upon nominal values.
96 hour LC50 = 14.9 mg/L (95% CI 9.91 to 20.0) based upon measured TC values.
Analytical method used was Total Carbon (TC). TC values represent the mean of samples taken on days 0, 2 and 4 less the control value, which was not reported. The LC50 values based upon TC and were re-calculated in 1994 and issued in an amended report.

Units/Value:

Results con't

- **Note: Deviations from protocol or guideline, analytical method, biological obsewations, control survival.**

Measured Conc. (mg/L of TC)	Fish Total Mortality (@96 hrs)
Control	0
1.39	0
2.71	0
4.90	0
9.91	0
19.86	20

*20 fish added at test initiation

Conclusion:

Reliability: (1) Reliable without restriction

Reference: BioDynamics Inc. 1985. A Flow-Through Acute Fish Toxicity Test. Study #230341.

Other (source): ExxonMobil Chemicals

Invertebrate Acute Toxicity

Test Substance:	CAS No.108419-32-5; C7 - C9 branched alkyl acetate ester
Method/Guideline:	USEPA TSCA
Year (guideline)	1992
Type (test type):	A Flow-Through Daphnia Acute Toxicity Test
GLP:	Yes
Year (study performed):	1985
Species:	Water Flea (Daphnia magna)
Analytical Monitoring:	Yes (TC)
Exposure Period:	48 hour
Statistical Method:	Finney, D.J. probit procedure of SAS

Test Conditions:

- **Note: Concentration prep.,** vessel **type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

A stock water accommodated fraction (WAF) was prepared by combining test substance with laboratory dilution water, at a ratio of 6.7ml per liter of water. The total volume prepared was not reported. The mixture was stirred for 72 hours and the 100% WAF was drawn out via a siphon tube and used for testing. The WAF was administered to the test chambers via a diluter system. The diluter system comprised of glass, stainless steel, with no plasticized materials. The diluter prepared the following test treatment levels: control, 6.25, 12.5, 25.0, 50.0, and 100.0 % WAF, which measured: NA, 1.87, 4.13, 10.24, 20.21, and 39.95mg /L as Total Carbon (TC). The test chambers were glass tanks with approximately 6L of test solution flowing through over a 24-hour period. Two replicates with ten daphnids each were tested per treatment level.
Test temperature was 21.36 +/- 0.39 Deg. C. Lighting was 16 hours dark and 8 hour light with gradual on/off periods and an intensity of 83 to 87 ft candles.
Dilution water hardness was 157 mg/L measured as $CaCO_3$. Dissolved oxygen was 7.9 to 8.8mg/L. The pH ranged from 7.5 to 8.1.

Organisms were supplied by in-house cultures; age = <24 hours old.

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

48 hour EC50 = 73.58 % WAF (95% Cl 62.18 to 89.3 % WAF) based upon nominal values.
48 hour EC50 based upon measured values was 29.4 mg TC/L. (95% Cl 24.6 to 36.3 mg TC/L)
Analytical method used was Total Carbon (TC). Measured TC values are based upon the mean of samples taken on days 0, 1 and 2 less the control value.

Meas. Conc. (mg TC/L)	Daohnia Total Mortality (@48 hrs)
Control	1
1.87	1
4.13	1
10.24	0
20.21	3
39.95	17

*20 Daphids total added at test initiation.
Mortality is defined as immobilized.
EC50 based upon TC is the result of a recalculation in an amended report in 1994.

Conclusion:

Reliability: (1) Reliable without restriction

Reference: BioDynamics, Inc. 1985. A Flow-Through Acute Daphnia Toxicity Test. Study # 230364.

Other (source): ExxonMobil Chemicals

Algal Toxicity

Test Substance:	CAS No. 108419-32-5, C7 - C9 branched alkyl acetate ester
Method/Guideline:	USEPA, Environmental Effects Test Guideline EPA 560/6-83-002
Year (guideline):	1983
Type (test type):	Algal Acute Toxicity Test
GLP:	Yes
Year (study performed):	1985
Species/Strain:	Fresh-Water Green Algae (Selenastrum capricornutum)
Analytical Monitoring:	Yes (TC, Total Carbon)
Exposure Period:	96 hour
Statistical Method:	Inverse interpolation method of Snedecor and Cochran
Test Conditions: • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organism culture, age.**	A Water Accommodated Fraction (WAF) stock solution was prepared by adding 6.7ml of test substance to 1 L of algal nutrient media in a 2L flask and mixed slowly for 72 hours. After mixing, the solution was transferred to a separatory funnel and allowed to settle for one hour. After settling, the solution was removed from the bottom and used as the 100% WAF. Individual treatments were prepared by diluting the 100% WAF with algal nutrient media. The test treatments were divided into 4 replicates. Three replicate were inoculated with algae at 2.0 x 1 0^4. The remaining replicate served as a blank. Treatment replicates were 125 ml erlenmeyer flasks containing 50 ml of solution. Flasks were placed on a shaker table during the study at -100 rpm. The test treatment concentrations were; control, 6.25, 12.5, 25, 50 and 100% WAF which measured, NA, 2.78, 5.74, 10.32, 21.46, and 44.71 mg TC/L respectively. Test temperature was 23.99 Deg. C. Lighting was continuous at -4300 Lux (400 ft candles). The pH was 7.5 at test initiation and ranged from 7.3 to 7.4 at test termination.
Results: **Units/Value:** **Measurement (cells/growth)**	72 hour EL50b=20.97mg TC/L (biomass) 72 hour EL50gr=29.65mg TC/L (growth rate) 96 hour EL50b=19.4mg TC/L (biomass) 96 hour EL50gr=43.52mg TC/L (growth rate) NOELRb = 31 .0 mg/L NOELRgr = 8.0 mg/L Analytical method used was Total Carbon (TC). Measured TC values are based upon Day 0 samples minus the control value (3.375mg TC/L). No excursions from the protocol were noted.

Results con't

Note: Deviations from protocol or guideline, analytical method, biological obsewations, control survival.

Nominal Conc (%WAF	Growth Rate 72 & 96 hr. (% Inhibition)		Mean Cell Conc. - 96 hr (cells/ml)
Control	na	na	$4.6x10^6$
6.25	0.11	1.59	4.0 xl 0^6
12.5	30.24	33.48	2.7 $x10^6$
25.0	2.50	3.33	3.6 $x10^6$
50.0	36.90	34.31	2.5 $x10^6$
100.0	63.51	60.48	1.8 $x10^5$

na - not applicable

Conclusion:

Reliability: (1) Reliable without restriction

Reference: Exxon Biomedical Sciences Inc. 1985. Algal Acute Toxicity Test. Study #230359.

Other (source): ExxonMobil Chemicals

Invertebrate Acute Toxicity

Test Substance:	CAS No.108419-34-7; C9 - Cl 1 branched alkyl acetate ester
Method/Guideline:	OECD 202
Year (guideline)	1984
Type (test type):	A Static Acute Daphnia Toxicity Test
GLP:	Yes
Year (study performed):	1999
Species:	Water Flea (Daphnia magna)
Analytical Monitoring:	Yes
Exposure Period:	48 hour
Statistical Method:	Trimmed Spearman Karber

Test Conditions:

- **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Individual treatment solutions were prepared as water accommodated fractions (WAFs). A WAF was prepared by adding test substance, via syringe, to 2.0L of laboratory dilution water in a glass aspirator bottle and mixing with a magnetic stir plate and bar. Mixing vortex was <10% of solution volume. After mixing for 24 hours at room temperature, the WAF was allowed to settle for one hour and removed from the port at the bottom of the bottle.
Test vessels were 125ml glass beakers filled with 140ml of solution and covered (no headspace). Four replicates were prepared for each treatment. Each replicate contained 5 organisms.
Nominal treatment levels were; control, 1.3, 3.2, 8.0, 20.0, and 50.0mg/ which measured; ND, 0.44, 1.3, 2.1, 1.9, 2.2mg/L respectively.
Test temperature was 20.0 Deg C. Lighting measured 691 Lux with 16 hrs light and 8 hrs dark. Dissolved oxygen ranged from 6.8 to 8.3mg/L. The pH ranged from 7.2 to 7.6.

Organisms were supplied by in-house cultures; age = <24 hours old. Parents age = 15 days old.

Results:

48 hour EL50 = 6.7mg/L (95% Cl 5.1 to 8.8) based upon nominal values.
48 hour EC50 based upon measured values was not reported.

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Analytical method used was GC-MSD. Measured values are based upon the mean of samples taken on day 0, and day 2.

Nominal. Conc. (mg/L)	Daphnia Total Mortality (@48 hrs)*
Control	0
1.3	0
3.2	4
8.0	11
20.0	19
50.0	20

*20 Daphids total added at test initiation.
Mortality is defined as immobilized.

Conclusion:

Reliability: (1) Reliable without restriction

Reference: Exxon Biomedical Sciences, Inc. 2000. Daphnia Acute Immobilization Test. Study # 129942.

Other (source): ExxonMobil Chemicals

Biodegradation

Test Substance: CAS No. 108419-34-7; C9 - Cl 1 branched alkyl acetate ester

Method/Guideline: OECD 301 F

Year (guideline): 1993

Type (test type): Ready Biodegradability, Manometric Respirometry Test

GLP: Yes

Year (study performed): 1995

Inoculum: Domestic activated sludge

Exposure Period: 28 days

Test Conditions:

- **Note: Concentration prep., vessel type, replication, test conditions.**

Test vessels were electronically monitored for oxygen consumption. Test material was tested in triplicate, while controls and blanks were tested in duplicate.
Test material concentration was approximately 45mg/L. Sodium benzoate (positive control) concentration was 50mg/L.
The inoculum was not acclimated.
All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.
Data were provided in a summary report, in which details of treatment preparation, media, vessel size, and temperature were not reported. However, the test procedure followed the OECD 301 F test guideline.

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

Test material was readily biodegradable. Half-life was 1 week. By day 28, 85% degradation of the test material was observed. 10% biodegradation was achieved on day 2, 50% biodegradation on approximately day 7.
By day 14, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted.
Biodegradation was based on oxygen consumption and the theoretical oxygen demand (ThOD) of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	81, 92, 81	84.7
Na Benzoate	92, 91	91.5

- replicate data

Conclusion:

Reliability:	(2) Reliable with restrictions
Reference:	Exxon Biomedical Sciences Inc. 1996 Ready Biodegradability, Manometric Respirometry. Study #1 29794A.
Other (source):	ExxonMobil Chemicals

Fish Acute Toxicity

Test Substance:	CAS No. 108419-35-8, Cl 1 - Cl4 branched alkyl acetate ester
Method/Guideline:	USEPA 40 CFR 792
Year (guideline):	N R
Type (test type):	Flow-Through Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1985
Species:	Fathead Minnow (Pimephales promelas)
Analytical Monitoring:	Yes (TC)
Exposure Period:	96 hour
Statistical Method:	Not Applicable
Test Conditions:	
- Note: **Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	A stock water accommodated fraction (WAF) was prepared by adding the test substance to laboratory blend water at a ratio of 1:150. The solution was stirred for 72 hours and the 100% WAF used for testing. The WAF was administered to the test chambers via a diluter system. The diluter system comprised of glass, stainless-steel with no plasticized materials. The diluter prepared the following test treatment levels: control, 6.25, 12.5, 25.0, 50.0, and 100.0 % WAF. The test chambers were 15L glass tanks containing 14L of solution. Two replicates with ten fish each were tested per treatment level. Test temperature was 21.78 +/- 0.15 Deg C. Lighting was gradual on and off with 16 hours dark and 8 hour light with an intensity of 77 to 79 ft candles. Dilution water hardness was 158 mg/L as $CaCO_3$. The pH ranged from 7.6 to 8.0. Dissolved Oxygen ranged from 7.7 to 8.6 mg/L. Fish were supplied by in-house laboratory; age = 25 weeks; mean wt.=0.276g; mean total length=2.5cm; test loading=0.023g of fish/L per 24 hour period.

Results:

96 hour LL_0 = 5800 mg/L.

Units/Value:

Value calculated based upon test substance loading.

Results con't

The amount of TOC measured (less the control value) was too low to measure.

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Nominal Conc. (% WAF)	Fish Total Mortality (@96 hrs)
Control	0
6.25	0
12.5	0
25.0	0
50.0	0
100.0	0

*20 fish added at test initiation

Conclusion:

The test material is considered non-toxic at its level of water solubility.

Reliability:

(1) Reliable without restriction

Reference:

BioDynamics Inc. 1985. A Flow-Through Acute Fish Toxicity Test. Study #252141.

Other (source):

ExxonMobil Chemicals

Invertebrate Acute Toxicity

Test Substance:	CAS No.108419-35-8; Cl 1 - Cl4 branched alkyl acetate ester
Method/Guideline:	USEPA 560/6-82
Year (guideline)	1984
Type (test type):	A Static Acute Daphnia Toxicity Test
GLP:	Yes
Year (study performed):	1985
Species:	Water Flea (Daphnia magna)
Analytical Monitoring:	Yes
Exposure Period:	48 hour
Statistical Method:	Not Applicable
Test Conditions: • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**	A water accomodated fraction (WAF) was prepared as a stock solution and then diluted to prepare the individual treatment levels. The WAF was prepared by adding 16.75ml of the test substance to 2.5L of laboratory dilution water in a glass carboy and mixed with a magnetic stir plate and bar. After mixing for 72 hours, the 100% WAF was drawn out through a sampling tube. Test vessels were 400ml glass beakers filled with 250ml of solution and covered. Four replicates were prepared for each treatment. Each replicate contained 10 organisms. Nominal treatment levels were; control, 6.25, 12.5, 25.0, 50.0, and 100.0 % WAF. Test temperature was 20.92 Deg C. Lighting measured 78 to 85 ft. candles with 16 hrs light and 8 hrs dark. Dissolved oxygen ranged from 8.3 to 9.5mg/L. The pH ranged from 8.2 to 8.5 units. Organisms were supplied by in-house cultures; age = <24 hours old. Parents age = 13 days old.

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

48 hour $EL_{,,}$ = 5829 mg/L (based upon calculation of test substance loading.

Analytical method used was Total Carbon (TC). The measured TC values (less the controls) were within the variability of the analytical method.

Nominal. Conc. WAF)	Daphnia Total Mortality (@48 hrs)*
Control	0
6.25	0
12.5	0
25.0	0
50.0	0
100.0	0

*40 Daphids total added at test initiation.
Mortality is defined as immobilized.
Some daphnids observed swimming on the surface in all treatment levels.

Three trials of the study were performed to confirm study results. Trials 2 and 3 exhibited no toxicity (trial 1 **was** not reported). The third trial is documented here.

Conclusion:

Reliability: (1) Reliable without restriction

Reference: Exxon Biomedical Sciences, Inc. 1985. An Acute Static Daphnia Toxicity Test. Study # 252142A.

Other (source): ExxonMobil Chemicals

Algal Toxicity

Test Substance:	CAS No. 108419-35-8, Cl 1 - Cl4 branched alkyl acetate ester
Method/Guideline:	USEPA, EPA 560/6-83-002
Year (guideline):	1983
Type (test type):	Algal Acute Toxicity Test
GLP:	Yes
Year (study performed):	1985
Species/Strain:	Fresh-Water Green Algae (Selenastrum capricornutum)
Analytical Monitoring:	Yes (TC, Total Carbon)
Exposure Period:	96 hour
Statistical Method:	Not Applicable
Test Conditions: • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organism culture, age.**	A Water Accommodated Fraction (WAF) stock solution was prepared by adding 6.7ml of test substance to 1 L of algal nutrient media (AAP) in a 2L flask and mixed slowly for 72 hours. After mixing, the solution was transferred to a separator-y funnel and allowed to settle for one hour. After settling, the solution was removed from the bottom and used as the 100% WAF. Individual treatments were prepared by diluting the 100% WAF with algal nutrient media. The test treatments were divided into 4 replicates. Three replicate were inoculated with algae at 2.0 x 1 0^4. The remaining replicate served as a blank. Treatment replicates were 125 ml erlenmeyer flasks containing 50 ml of solution. Flasks were placed on a shaker table during the study at -100 rpm. The test treatment concentrations were; control, 6.25, 12.5, 25, 50 and 100% WAF which measured (less the control value) na, 0, 0.058, 0.219, 0.492, and 0.873ppm of TC. Test temperature was 23.89 Deg. C. Lighting was continuous at 400 ft candles. The pH was 7.5 at test initiation and ranged from 7.3 to 7.4 at test termination.
Results: **Units/Value:** **Measurement (cells/growth)**	96 hour EL_0b: = 5829 mg/L 96 hour EL_0gr: = 5829 mg/L NOELRb = 5829 mg/L NOELRgr = 5829 mg/L No Inhibition of Algal growth was observed at the highest treatment level 100% WAF (0.873 ppm Carbon). Concentration re-calculated based upon loading of test substance. Analytical method used was Total Carbon (TC). Measured TC values are based upon Day 0 samples less the control value on day 0 of the study. No excursions from the protocol were noted.

Results con't

Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.

Nominal Conc. (%WAF)	Mean Cell Conc. • 96 hr (cells/ml)
Control	5.2×10^6
6.25	4.4 xl 0^6
12.5	4.6 xl 0^6
25.0	4.1 $\times 10^6$
50.0	5.3 xl 0^6
100.0	5.2 xl 0^6

Conclusion:

Reliability: (1) Reliable without restriction

Reference: BioDynamics, Inc. 1985. An Acute Algal Toxicity Test. Study #252159.

Other (source): ExxonMobil Chemicals

Biodegradation

Test Substance:	CAS No. 108419-35-8; Cl 1 - Cl4 branched alkyl acetate ester
Method/Guideline:	USEPA EPA 560/6-83-003, CG-2000
Year (guideline):	1982
Type (test type):	Aerobic Aquatic Biodegradation
GLP:	Yes
Year (study performed):	1985
Inoculum:	Acclimated media
Exposure Period:	28 days
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The inoculum was acclimated to the test substance for 14 days prior to study initiation. The media consisted of mineral salt solutions, pond sediment, activated sludge, distilled water, and small amounts (10ul) of test substance. The media was mixed and placed on a gyrorotatory shaker in the dark for 13 days. After settling overnight the supernatant was pour off and was used as the inoculum for the test phase. The test system utilized 2.0L Glenhill flasks as test vessels. Approximately 13.0mg of test substance were added to 900ml of glass distilled water. Additionally, 1 00ml of acclimated media and 1 ml of mineral salts were added. The flasks were sealed and placed on a gyrorotatory shaker in the dark. Three replicates of the test substance were evaluated. Twice a week, the flasks were monitored for spent NaOH and titrated for carbon dioxide (CO_2). Total Organic Carbon (TOC) was measured at initiation and termination in the controls. A positive and negative control were tested consisting of Phthalic acid (100ml at 103.8mg/L) and HgC12 (10 ml at 51g/L) respectively, along with three blanks. Test temperature ranged from 21.5 to 25.0 Deg C.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	The test material was not readily biodegradable. By day 28, 31% degradation of the test material was observed. The half-life, and 10% biodegradation achievement periods were not reported. The positive control (phthalic acid) degraded by 43.8% by day 28, with a TOC removal of 100.7% Biodegradation was based on NaOH usage and calculated CO_2 evolution. No excursions from the protocol were noted.
Conclusion:	

Reliability:	(2) Reliable with restrictions TOC values not measured on test treatments only controls. No replicate values reported (mean only).
Reference:	BioDynamics, Inc. 1985 Ultimate Biodegradability, Study # 252189
Other (source):	ExxonMobil Chemicals