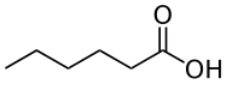
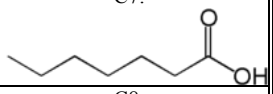
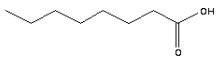
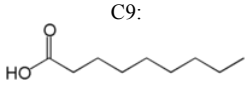
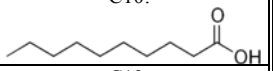
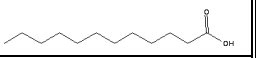
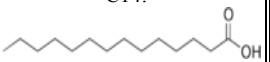
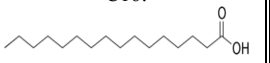
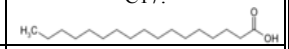
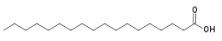
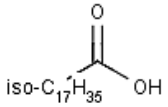
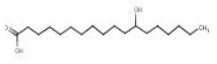
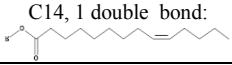
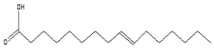
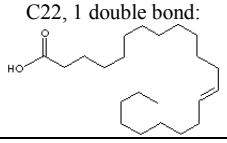
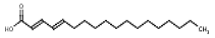
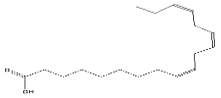
SIDS INITIAL ASSESSMENT PROFILE

Category name	Aliphatic Acids Category

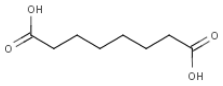
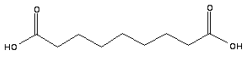
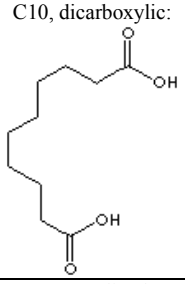
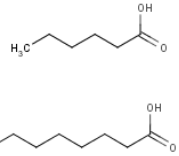
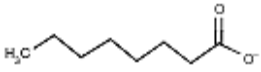
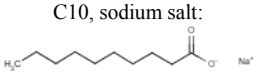
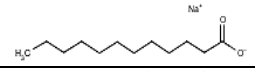
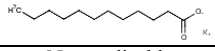
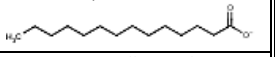
CAS No(s), Chemical name(s) and structural formula(s) [1]

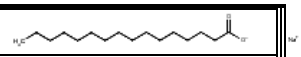
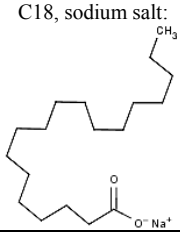
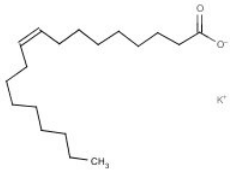
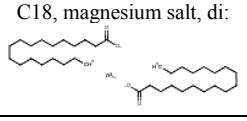
CAS No	IUPAC or CAS Name	Structural Formula
Single component – Saturated (12)		
142-62-1	Hexanoic acid	C6: 
111-14-8	Heptanoic acid	C7: 
124-07-2	Octanoic acid	C8: 
112-05-0	Nonanoic acid	C9: 
334-48-5	Decanoic acid	C10: 
143-07-7	Dodecanoic acid	C12: 
544-63-8	Tetradecanoic acid	C14: 
57-10-3	Hexadecanoic acid	C16: 
506-12-7	Heptadecanoic acid	C17: 
57-11-4	Octadecanoic acid	C18: 
30399-84-9	Isooctadecanoic acid	C18, methyl branched: 
106-14-9	12-Hydroxyoctadecanoic acid; 12-hydroxy-octadecanoic acid	C18, 1 hydroxyl group: 
Single component – Mono- unsaturated (4)		
544-64-9	(Z)-Tetradec-9-enoic acid; 9-Tetradecenoic acid, (Z)-	C14, 1 double bond: 
2091-29-4	9-Hexadecenoic acid, (Z)-	C16, 1 double bond: 
112-80-1	(Z)-Octadec-9-enoic acid; 9-Octadecenoic acid, (Z)-	C18, 1 double bond:

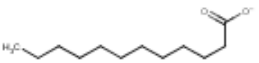
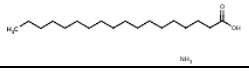
[1] The table is organized according to general aliphatic acid structure. Specifically, by increasing carbon chain length, with any structure variations (e.g., unsaturated, dicarboxylic, double bonds, hydroxyls, salts) appearing after the corresponding base structure.

		
112-86-7	(Z)-Docos-13-enoic acid; 13-Docosenoic acid, (Z)-	C22, 1 double bond: 
Single component - Di-unsaturated (2)		
60-33-3	(9Z,12Z)-Octadeca-9,12-dienoic acid; 9,12-Octadecadienoic acid	C18, 2 double bonds: 
121250-47-3	(8E,12E)-octadeca-8,12-dienoic acid; Octadecadienoic acid (Conjugated linoleic acid)	C18, 2 adjacent double bonds: 
Single component - Tri-unsaturated (1)		
463-40-1	(9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid; 9,12,15-Octadecatrienoic acid, (Z,Z,Z)	C18, 3 double bonds: 
Alkyl range sourced based (multi-component) – Saturated (13)		
68603-84-9[2]	Carboxylic acids, C5-9	Not Applicable
68937-74-6	Fatty acids, C6-10	Not Applicable
67762-36-1	Fatty acids, C6-12	Not Applicable
68937-75-7	Fatty acids, C8-10	Not Applicable
90990-08-2	Fatty acids, C8-18	C12-14
68002-90-4	Fatty acids, C10-16	Not Applicable
90990-10-6	Fatty acids, C12-14	Not Applicable
67701-01-3	Fatty acids, C12-18	Not Applicable
67701-02-4	Fatty acids, C14-18	Not Applicable
68424-37-3	Fatty acids, C14-22	Not Applicable
67701-03-5	Fatty acids, C16-18	Not Applicable
68937-76-8	Fatty acids, C16-20	Not Applicable
90990-11-7	Fatty acids, C18-22	Not Applicable
Alkyl range sourced based (multi-component) –Unsaturated (1)		
68648-24-8	Fatty acids, vegetable-oil, unsaturated	Not Applicable
Alkyl range sourced based (single or multi-component) – Mixture of saturated and unsaturated (16)		
68937-85-9	Fatty acids, coco, heavy fractions	Not Applicable
68938-15-8	Fatty acids, coco, hydrogenated	Not Applicable
61788-47-4	Fatty acids, coco	Not Applicable
67701-05-7	Fatty acids, C8-18 and C18-unsaturated	Not Applicable
68918-39-8	Soaps, stocks, C8-18 and C18 unsaturated alkyl, acidulated	Not Applicable
90990-15-1	Fatty acids, C12-18 and C18-unsaturated	Not Applicable
68334-03-2	Fatty acids, C12-20 and C12-20 unsaturated	Not Applicable
61790-38-3	Fatty acids, tallow, hydrogenated	Not Applicable
67701-06-8	Fatty acids, C14-18 and C16-18-unsaturated	Not Applicable

[2] Multi-component substances are presented in red text.

61790-37-2	Fatty acids, tallow	Not Applicable
68308-53-2	Fatty acids, C14-18 and C16-18-unsaturated, sodium salts	Not Applicable
68002-87-9	Fatty acids, C14-18 and C16-22-unsaturated	Not Applicable
68440-15-3	Fatty acids, palm-oil	Not Applicable
67701-07-9	Fatty acids, C16 and C18-unsaturated	Not Applicable
67701-08-0	Fatty acids, C16-18 and C18-unsaturated	Not Applicable
61789-45-5	Fatty acids, dehydrated castor-oil	Not Applicable
Dicarboxylic acids (single or multi-component) Saturated (4)		
68937-72-4	Carboxylic acids, di-, C4-11	C6-9, dicarboxylic 
123-99-9	Nonanedioic acid	C9, dicarboxylic: 
111-20-6	Decanedioic acid	C10, dicarboxylic: 
68937-70-2	Carboxylic acids, C6-18 and C8-15 di-	C9-18; C6-14, dicarboxylic: 
Sodium and potassium salts (single or multi-component) Saturated (10)		
67762-44-1	Fatty acids, C6-12, Na salts	Not applicable
1984-06-1	Sodium octanoate; Octanoic acid, sodium salt	C8, sodium salt: 
1002-62-6	Sodium decanoate; Decanoic acid, sodium salt	C10, sodium salt: 
629-25-4	Sodium dodecanoate; Dodecanoic acid, sodium salt	C12, sodium salt: 
10124-65-9	Potassium dodecanoate, Dodecanoic acid, potassium salt	C12, potassium salt: 
91032-12-1	Fatty acids, C12-18, sodium salts	Not applicable
822-12-8	Sodium tetradecanoate; Tetradecanoic acid, sodium salt	C14, sodium salt: 
408-35-5	Sodium hexadecanoate; Hexadecanoic acid, sodium	C16, sodium salt:

	salt	
68424-38-4	Fatty acids, C16-18, sodium salts	Not applicable
822-16-2	Sodium octadecanoate; Octadecanoic acid, sodium salt	C18, sodium salt: 
Sodium and potassium salts (single component) Mono-unsaturated (1)		
143-18-0	Potassium (Z)-octadec-9-enoate; 9-Octadecenoic acid, (Z)-, potassium salt	C18, 1 double bond, potassium salt: 
Sodium and potassium salts (multi-component) Mixture of saturated and unsaturated (9)		
61789-30-8	Fatty acids, coco, potassium salts	Not applicable
61789-31-9	Fatty acids, coco, sodium salts	Not applicable
67701-09-1	Fatty acids, C8-18 and C18-unsaturated, potassium salts	Not applicable
67701-10-4	Fatty acids, C8-18 and C18-unsaturated, sodium salts	Not applicable
68082-64-4	Fatty acids, vegetable-oil, sodium salts	Not applicable
67701-11-5	Fatty acids, C14-18 and C16-18-unsaturated, sodium salts	Not applicable
8052-48-0	Fatty acids, tallow, sodium salts; Fatty acids, tallow, sodium salts	Not applicable
61790-79-2	Fatty acids, palm-oil, sodium salts	Not applicable
68002-80-2	Fatty acids, C14-18 and C16-18-unsaturated, potassium salts	Not applicable
Magnesium and calcium salts (multi-component) - Mixture Saturated and Unsaturated (1)		
64755-01-7	Fatty acids, tallow, calcium salts	Not applicable
Magnesium and calcium salts (single component) Saturated (2)		
542-42-7	Calcium hexadecanoate; Hexadecanoic acid, calcium salt	C16, calcium salt
557-04-0	Magnesium octadecanoate; Octadecanoic acid, magnesium salt	C18, magnesium salt, di: 

Ammonium salts (single component) Saturated (2)		
2437-23-2	Azanium dodecanoate; Dodecanoic acid, ammonium salt	C12, ammonium salt: 
1002-89-7	Azanium octadecanoate; Octadecanoic acid, ammonium salt	C18, ammonium salt: 

SUMMARY CONCLUSIONS OF THE SIAR

Analogue/Category Rationale

The aliphatic acids category consists of 78 sponsored naturally derived (from plant or animal fats and oils) homologous aliphatic acids, 74 contain a carboxyl group at the polar end, while the nonpolar tail of the molecule consists of a hydrocarbon chain; an additional four (4) contain a carboxyl group at both ends and the non-polar hydrocarbon chain in the middle. Fatty acids are amphiphilic compounds; in other words, each molecule has a hydrophilic, polar part (the carboxyl group) and a hydrophobic, nonpolar part (the hydrocarbon tail). The aliphatic acids category consists of C4-C22 aliphatic acids, also called fatty acids, and their salts. All naturally occurring unsaturated fatty acids (plant and animal derived) are cis isomers; trans-unsaturated aliphatic acids are not included in the category. Substances that are source named are derived from the stipulated source material. For example, coco fatty acid means the source is coconut oil; tallow specifies animal fat, etc. The specific source for substances that are not source named (for example, **Fatty acids, C16-18 and C18-unsaturated**[3]) cannot be stipulated, but the source is plant or animal fats or oils. The sponsored substances may be saturated, unsaturated or a mixture of saturated and unsaturated aliphatic chains. The sponsored aliphatic acids include single carbon chain length substances (single component aliphatic acids), homologous mixtures of the single carbon chain length substances (multi-component aliphatic acids), homologous salts of the single and multi-component substances and single carbon chain length dicarboxylic acids, and di-acid salts of the single component substances. The single component substances include saturated compounds and mono-, di- or tri-unsaturated compounds. The multi-component substances include saturated, unsaturated and undefined mixtures of saturated and unsaturated carbon chains. The level of unsaturation cannot be described as these are naturally derived, not pure substances, and the substance descriptors do not allow for differentiation at the level of unsaturation. The sodium salts include single and multi-component saturated compounds and multi-component, mixture of saturated and unsaturated compounds. The potassium salts include saturated, single component mono-unsaturated and multi-component

[3] Sponsored substances are presented in **bold** text.

mixture of saturated and unsaturated compounds. The ammonium salts are single component saturated compounds. The magnesium or calcium di-acids are two single component saturated acid chains associated with one metal ion.

The general structure for aliphatic (mono) acids is:
RC(=O)OX, where:
R is a linear alkyl chain that may be saturated or unsaturated (with 1 to 3 double bonds) and;
X is a hydrogen ion; or X = the ammonium, sodium, potassium, magnesium or calcium ion for salts.
(Note: Salts of calcium and magnesium are "+2"; they can form salts with two carboxylic acid chains while sodium and potassium which are "+1", form salts with only a single acid chain.)

Notable structural features of individual category members that vary from the general structure above include a methyl branched substance, a hydroxyl group substituted substance, and the dicarboxylic acids.

A methyl-branched single component saturated aliphatic acid (**isooctadecanoic acid; CAS 30399-84-9**) is not a highly branched material, rather the branching is a minor variation on a long aliphatic acid chain, and the branching is not expected to affect the properties of the substance.

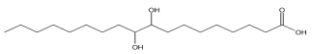
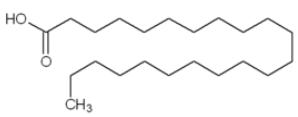
A single component saturated aliphatic acid contains a hydroxyl group (**12-hydroxy-octadecanoic acid, CAS 106-14-9**); this additional side chain is not a functional group on the molecule and is not expected to affect the properties of the substance.

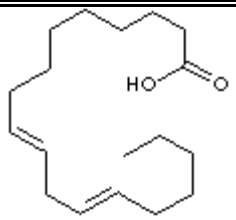
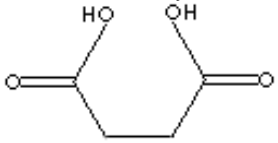
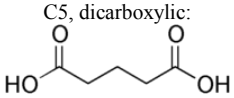
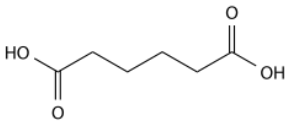
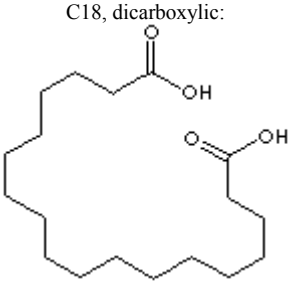
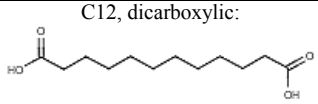
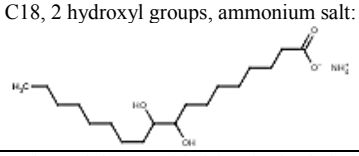
Sponsored substances also include single-chain length and multi-component chain length dicarboxylic acids; the dicarboxylic acids have no structural differences in functional groups.

Analogues: An additional fourteen (14) aliphatic acids are included as supporting substances and are distributed among the same subgroups as the sponsored substances.

Key points are that the sponsored and supporting substances share:
- The same structural features
- Similar metabolic pathways
- Common mode of ecotoxicological action
- Common levels and mode of human health related effects.

Identity of the supporting substances

CAS No	IUPAC or CAS Name	Molecular Formula [(a)]	Structural Formula	Molecular Weight [(1)]
Single component				
120-87-6	9,10-Dihydroxy-octadecanoic acid	C18-H36-O4	C18, 2 hydroxyl groups: 	316.49
112-85-6	Docosanoic acid	C22-H44-O2	C22: 	340.6
2197-37-7	(9Z,12Z)-octadeca-9,12-dienoic acid; 9,12-Octadecadienoic acid	C18-H32-O2	C18, 2 double bonds:	280.45

				
Alkyl ranges and sourced based				
95912-82-6	Fatty acids, C16-22 and C18-22 unsaturated	Not applicable	C16-22, unsaturated	Not applicable
61790-12-3	Fatty acids, tall-oil	Not applicable	C18, 1 double bond (predominately); C18-20	Not applicable
85711-54-2	Fatty acids, rape-oil	Not applicable	C18-22	Not applicable
68953-27-5	Fatty acids, sunflower, conjugated	Not applicable	C16-18, adjacent double bonds	Not applicable
Dicarboxylic acids				
110-15-6	Butanedioic acid	C4-H6-O4	C4, dicarboxylic: 	118.09
110-94-1	Pentanedioic acid	C5-H8-O4	C5, dicarboxylic: 	132.12
124-04-9	Hexanedioic acid	C6-H10-O4	C6, dicarboxylic: 	146.14
871-70-5	Octadecanedioic acid	C18-H34-O4	C18, dicarboxylic: 	314.47
693-23-2	Dodecanedioic acid	C12-H22-O4	C12, dicarboxylic: 	230.31
Sodium and potassium salts (2)				
68424-26-0	Fatty acids, C16-18 and C18-unsaturated, sodium salts	Not applicable	C16-22, unsaturated, sodium salts	Not applicable
Ammonium salts (2)				
84753-04-8	9,10-Dihydroxy-octadecanoic acid, ammonium salt	C18-H36-O4.H3-N	C18, 2 hydroxyl groups, ammonium salt: 	333.52

(1) Molecular formula not available for multi-component substances. Molecular weights provided for single chain length aliphatic acids.
(2) Sodium, potassium, magnesium, calcium and ammonium aliphatic acid salts contain the same chain length (or range) as a

corresponding single component or Alkyl range or source based sponsored substance. As such, read across to the corresponding sponsored substances or supporting substances is reasonable.

The supporting substances are used to supplement existing human health and environmental data for the sponsored substances.

Summary of supporting substance human health read across data

Substance	Irritation		Acute toxicity	Repeated dose toxicity	Mutagenicity	Fertility and Development
	Skin	Eye				
Single Component						
120-87-6	NO DATA	X	NO DATA	NO DATA	NO DATA	NO DATA
112-85-6	NO DATA	NO DATA	X	X	X	X
Alkyl Range Source based						
61790-12-3	NO DATA	NO DATA	X	X	X	X
85711-54-2	NO DATA	NO DATA	X	NO DATA	NO DATA	NO DATA
Dicarboxylic acids						
110-15-6	X	X	X	X	X	NO DATA
110-94-1	X	X	X	X	X	X
124-04-9	X	X	X	X	X	X
693-23-2	NO DATA	NO DATA	X	X	X	X
871-70-5	NO DATA	X	X	X	X	NO DATA
Sodium and Potassium salts						
68424-26-0	NO DATA	NO DATA	X	NO DATA	NO DATA	NO DATA
Ammonium salts						
84753-04-8	X	X	X	NO DATA	X	NO DATA

X= data available and used for read across

Summary of supporting substance environmental read across data

Substance	Biodegradation	Acute toxicity		
		Fish	Daphnia	Algae
Single Component				
120-87-6	NO DATA	X	NO DATA	NO DATA
Alkyl Range Source based				
95912-82-6	NO DATA	NO DATA	X	NO DATA
68953-27-5	NO DATA	X	NO DATA	NO DATA
Dicarboxylic acids				
110-15-6	NO DATA	NO DATA	X	NO DATA
124-04-9	NO DATA	X	X	NO DATA
693-23-2	NO DATA	NO DATA	NO DATA	X
871-70-5	NO DATA	X	X	X
Sodium and Potassium salts				
91302-02-9	X	NO DATA	NO DATA	NO DATA
68424-26-0	NO DATA	X	NO DATA	NO DATA

X= data available and used for read across

The aliphatic acids share a common degradation pathway in which they are metabolized to acetyl-CoA or other key metabolites in all living systems. Common biological pathways result in structurally similar breakdown products, and are, together with the physico-chemical properties, responsible for similar environmental behavior and essentially identical hazard profiles with regard to human health. Differences in metabolism or biodegradability of even and odd numbered carbon chain compounds or saturated/unsaturated compounds are not expected; even- and odd- numbered carbon chain compounds, and the saturated and unsaturated compounds are naturally occurring and are expected to be metabolized and biodegraded in the same manner.

The acid and alkali salt forms of the homologous aliphatic acid are expected to have many similar physicochemical and toxicological properties when they become bioavailable; therefore, data read across is used for those instances where data are available for the acid form but not the salt, and vice versa. In the gastrointestinal tract, acids and bases are absorbed in the undissociated (non-ionized) form by simple diffusion or by facilitated diffusion. It is expected that both the acids and the salts will be present in (or converted to) the acid form in the stomach. This means that for both aliphatic acid or aliphatic acid salt, the same compounds eventually enter the small intestine, where equilibrium, as a result of increased pH, will shift towards dissociation (ionized form). Hence, the situation will be similar for compounds originating from acids and therefore no differences in uptake are anticipated.

Given the large number of substances in this category, their closely related chemical structure, expected trends in physical chemical properties, and similarity of toxicokinetic properties, both mammalian and aquatic endpoints were filled using read-across to the closest structural analogue, and selecting the most conservative sponsored or supporting substance effect level (see Tables 1, 2 and 3 at the end of this document). Structure-activity relationships are not evident for the mammalian toxicity endpoints. That is, the low mammalian toxicity of this category of substances limits the ability to discern structural effects on biological activity. Regardless, the closest structural analogue with the most conservative effect value was selected for read across. Irritation is observed for chain lengths up to a "cut-off" at or near 12 carbons). Structure-activity relationships based on carbon chain length are evident in the available data on the aquatic ecotoxicity of substances of this category (aquatic toxicity increases with increasing chain length up to a "cut-off" at or near 12 carbons). Read-across between the (sponsored and supporting) subgroups and the category as a whole was used for the human health and environmental endpoints. Read across can be made between all sponsored substances (without regard for subcategory), and the lowest effect value for the closest structural analogue is selected.

The closest structural analogue was identified, and this approach has been used as the basis for the read across for human health endpoints. The closest structural analogues were ordered for each subdivision (using ">" to indicate the order of read across used), and the most conservative effect value for the closest structural analogue was selected to fill data gaps. The order of closest structural analogue follows for each subdivision. Note that the saturation or unsaturation level is not a factor in the toxicity of these substances and is not a critical component of the read across process. Where possible, we have prioritized read across between similar states of saturation and unsaturation. Higher water solubility of the potassium, sodium and ammonium salts make these a lower ranked analogy for the (non-salt) aliphatic acids, while lower water solubility of the magnesium and calcium salts make these a lower ranked analogy for all other members of the category.

Single Component (saturated and unsaturated) is read across to any other Single component > Alkyl Range Source Based > Sodium, Potassium, and Ammonium salts> Dicarboxylic acids> Magnesium and calcium salts.
Alkyl Range Source Based (saturated and unsaturated) is read across to any other Alky Range Source Based >Single component > Sodium, Potassium, and Ammonium salts> Dicarboxylic acids> Magnesium and calcium salts.
Dicarboxylic acids (saturated) is read across to any other Dicarboxylic acids > Single component or Alkyl Range Source Based > Dicarboxylic acids> Magnesium and calcium salts.
Sodium and Potassium salts (saturated and unsaturated) is read across to any other Sodium and Potassium salts > Ammonium salts > Single component or Alkyl Range Source Based > Dicarboxylic acids> Magnesium and calcium salts.
Magnesium and calcium salts (saturated and unsaturated) is read across to any other Magnesium and calcium salts > Single component or Alkyl Range Source Based > Dicarboxylic acids > Sodium, Potassium, and Ammonium salts.
Ammonium salts (saturated) is read across to any other Ammonium salts > Sodium or Potassium salts> Single component or Alkyl Range Source Based > Dicarboxylic acids > Magnesium and calcium salts.

Determination of closest structural analogue for aquatic toxicity endpoints. Clear trends for water solubility were driven by carbon chain length and by type of salt (see carbon chain length/water solubility trend tables). Therefore, the closest structural analogue definition for aquatic toxicity took into account not only closest structural analogue as described above for human health, but also consideration of similarity of carbon chain length or salt (and thus corresponding water solubility), before selection of the most conservative effect value to fill data gaps. In cases where the corresponding carbon chain length substances did not have data, the closest chain

length was selected, using a conservative (lowest value) approach.

Higher water solubility of the potassium, sodium and ammonium salts make these a lower ranked analogy for the aquatic toxicity endpoints for the (non-salt) aliphatic acids (and vice versa), while lower water solubility of the magnesium and calcium salts make these a lower ranked analogy for all other members of the category.

Single Component (saturated and unsaturated) is read across based on carbon chain length to other Single components > Alkyl Range Source Based > Dicarboxylic acids > Sodium, Potassium, and Ammonium salts > Magnesium and calcium salts.
Alkyl Range Source Based (saturated and unsaturated) is read across based on carbon chain length of Alkyl Range Source Based >Single component using the lowest carbon chain length of the mixture > Dicarboxylic acids > Sodium, Potassium, and Ammonium salts > Magnesium and calcium salts.
Dicarboxylic acids (saturated) is read across to any other Dicarboxylic acids > based on carbon chain length to Single component > Alkyl Range Source Based > Sodium, Potassium, and Ammonium salts> Magnesium and calcium salts.
Sodium and Potassium salts (saturated and unsaturated) is read across to any other Sodium and Potassium salts > Ammonium salts > based on carbon chain length to Dicarboxylic acids > Single component or Alkyl Range Source Based > Magnesium and calcium salts.
Magnesium and calcium salts (saturated and unsaturated) is read across to any other Magnesium and calcium salts > based on carbon chain length to Single component or Alkyl Range Source Based > Dicarboxylic acids > Sodium, Potassium, and Ammonium salts.
Ammonium salts (saturated) is read across to any other Ammonium salts > Sodium or Potassium salts> based on carbon chain length to other Dicarboxylic acids > Single component or Alkyl Range Source Based > Magnesium and calcium salts.

Physical-chemical Properties

Sponsored substances include single chain length aliphatic acids and mixtures of defined chain length ranges of aliphatic acids. Physical-chemical property estimates are for a discrete chain length as the estimation technique is based on a relationship between a specific chemical structure and a measured or estimated property of that structure. A property of a mixture of aliphatic acids is therefore a function of that property for each of the discrete chain length components in the mixture.

With regard to the physical / chemical properties of the sponsored Aliphatic Acids, two predominant trends are clearly evident with increasing alkyl chain length and include: i) increasing melting point, boiling point, and partition coefficient, and ii) decreasing water solubility and vapour pressure. Within a given carbon chain length, melting point increases with increasing saturation and decreases with increasing unsaturation. For example, 9-Octadecenoic acid, (Z)- (CAS 112-80-1) is mono-unsaturated and is a liquid; **Octadecanoic acid (CAS 57-11-4)** is saturated and is a solid. These trends are clearest to identify within each subgroup of Aliphatic Acids (single component - saturated, single component - unsaturated; alkyl range sourced - saturated, etc.). Within a given subgroup, when these trends are not clear, it is due to the comparison between measured and modeled data. When the comparison is repeated to compare between modeled estimates, the trends observed with increasing carbon chain length remain applicable. The following text and tables are organized by subdivision and describe these trends in more detail.

- **Single component**: The noted general trends with increasing alkyl chain length are observed when the entire single component group (12 saturated, 4 mono-unsaturated, 2 di-unsaturated, and 1 tri-unsaturated substances) is evaluated together; that is, the degree of saturation or unsaturation does not alter the properties trend. The effect of mono-unsaturation (C14:1 to C22:1) appears to be a slight increase in water solubility and a slight decrease in the partition coefficient, as compared to the corresponding saturated substances; a similar trend is noted for the C18 di- or tri-unsaturated. Slight (although inconsistent) effects on the trend for decreasing vapor pressure are also are also observed with the mono-, di- and tri-unsaturated substances as compared to the corresponding saturated substances.
- **Alkyl range sourced**: When considering the properties of the individual (single chain length) components, the two predominant trends [i) increasing melting point, boiling point, and partition coefficient, and ii) decreasing water solubility and vapour pressure] are evident with increasing alkyl chain length. Also

apparent are the slight effects of unsaturation, as noted above for the single component substances.

- **Dicarboxylic acids**: Compared to their corresponding single acid substances (C8-10 single component, saturated), the dicarboxylic acids exhibit modestly higher melting / boiling points and water solubility, and lower partition coefficients and vapour pressures. The trends described above for changes in physical chemical properties with increasing carbon chain length apply.

- **Salts**: As expected, the salts differ in physical / chemical properties as compared to their homologous single component substances. However the trends described above for single components with regard to changes in physical chemical properties with increasing carbon chain length apply.

Physical Chemical Property Trend Analysis by Subcategory

SUMMARY SINGLE COMPONENT					
Increasing Carbon chain	Melting point (ºC)	Boiling point (ºC at 1013 hPa)	Partition coefficient (log Kow) (--)	Water Solubility (mg/L at 25ºC)	Vapor pressure (hPa at 25 ºC)
Single Component: Saturated (12)					
Increasing C chain, C6-18	Increases (-3 - 152.85)	Increases (205.2 - 414.8)	Increases (1.92 - 8.23)	Decreases (1E+4 - 10^{-3})	Decreases (10^{-3} - 10^{-9})
Single Component: Mono-Unsaturated (4)					
C14-22, mono-unsaturated	No pattern across measured & modeled; Increases across modeled (99.5 - 158.97)	Increases (339 - 432.03)	Increases (5.8 - 9.69)	Decreases (0.94 - 10^{-5})	Decreases (10^{-5} - 10^{-7})
Single Component: Di-Unsaturated (2)					
C18, di-unsaturated	Increases across measured / modeled (-8.5 - 132.4); Same modeled (132.4)	Similar across measured / modeled (365.2 - 389.2); Same modeled (389.2)	Similar across measured / modeled (7.05 - 7.51); Same modeled (7.51)	Same, both modeled (0.0377)	Increases across measured / modeled (10^{-6} - 10^{-5}); Same modeled (10^{-5})
Single Component: Tri-Unsaturated (1)					
C18, tri-unsaturated	-16.5	231	6.46	0.124	10^{-7}
SUMMARY Alkyl range sourced based					
Alkyl Range Sourced Based (Multi-Component): Saturated (13)					
C5-9 - C18-22	Increases (-3 - 81)	Increases (205.2 - 383)	Increases (1.92 - 9.91)	Decreases (10^{4} - 10^{-4})	Decreases (10^{-2} - 10^{-7})
Alkyl Range Sourced Based (Multi-Component): Unsaturated (1)					
C12-20, mono-unsaturated	Decreases across measured / modeled (88.3 – 23); Increases across modeled (88.3 – 149.21)	Increases (313.1-408.8)	Increases (4.78-8.71)	Decreases (9.12 - 10^{-4})	Decreases (10^{-4} – 10^{-6})
Alkyl Range Sourced Based (Multi-Component): Mixture of saturated and unsaturated (16)					
C8-20	Increases (16.3 - 75.4)	Increases (239-383)	Increases (3.05 - 9.29)	Decreases (789 - 10^{-4})	Decreases (10^{-3} - 10^{-9})
C18 – C22, mono-unsaturated (1)	Increases (13.4 - 33.5) (1)	Increases (360 - 432) (1)	Increases (7.64 - 9.69) (1)	Decreases (0.0115 – 10^{-5}) (1)	No pattern across measured & modeled; Decreases across modeled (10^{-5} - 10^{-6}) (1)
SUMMARY Dicarboxylic acids					
Increasing C chain	MP (ºC)	BP (ºC at 1013 hPa)	Partition coefficient (--)	Water Solubility (mg/L at 25ºC)	Vapor pressure (hPa at 25 ºC)
Dicarboxylic Acids (Single- or Multi-Component): Saturated (4)					
C8 - C10, di' (2)	No pattern across measured / modeled; Small increase across modeled (119.13 - 127.36) (2)	No pattern across measured / modeled; Small increase across modeled (336.56 - 360.05) (2)	Increases (1.21 - 2.19) (2)	Decreases (10^{4} - 1000) (2)	Decreases (10^{-7} - 10^{-8}) (2)
SUMMARY Sodium and potassium salts					
Sodium and Potassium Salts (Single- or Multi-Component): Saturated (10)					
C6-18	Increases (172.6 - 286.5)	Increases (438.8 - 578.0)	Increases (-2.17 - 4.13)	Decreases (10^{6} - 3.32)	Decreases (10^{-8} - 10^{-12})

Sodium and Potassium Salts (Single-Component): Unsaturated (1)					
C18, mono-unsaturated	250.71	581.6	3.9	4.19	1.04 E-12
Sodium and Potassium Salts (Multi-Component): Mixture of Saturated and Unsaturated (9)					
C8-18	Increases (188.0 - 249.0)	Increases (462 - 578)	Increases (-1.38 - 4.13)	Decreases (10^{5} - 3.32)	Decreases (10^{-9} - 10^{-12})
C18, mono- and di-unsaturated [3]	Increases (233.5 - 252.4) [3]	Small increase (581.6 - 585.2) [3]	Decreases (3.92 - 3.70) [3]	Increases (5.21 - 8.17) [3]	Decreases (10^{-12} - 10^{-13}) [3]
SUMMARY Magnesium and calcium salts					
Magnesium and Calcium Salts (Single- or Multi-Component): Saturated or Mixture Saturated and Unsaturated (3)					
C14-18, magnesium and calcium salts	Increases 231.9 - 287.83)	Increases (568.2 - 661.1)	Increases (10.41 - 14.34)	Decreases (10^{-7} - 10^{-10})	Decreases (10^{-12} - 10^{-15})
C18, mono-unsaturated, calcium salt	291.2	668.2	13.91	10^{-10}	10^{-15}
SUMMARY Ammonium salts					
Ammonium Salts (Single Component): Saturated (2)					
C12-18, ammonium salts	Increases across modeled (180.71 - 213.23)	Increases (491.71 - 501.4)	Increases (2.12 - 5.07)	Decreases (547.8 - 0.565)	Decreases ($4 \times 10^{-8} – 3 \times 10^{-8}$)

[1] Comparing across the mono-unsaturated CAS (C18:1, C20:1, and C22:1)
[2] Excluding **68937-70-2** which was not modeled as a dicarboxylic acid
[3] Carbon chain length the same; range reflects differing levels desaturation

The trends for water solubility were also examined by carbon chain length across the sponsored aliphatic acid subdivisions, and for the homologous salts. In general, the water solubility of single carbon chain length substances followed a pattern of decreasing solubility as carbon chain length increases, especially at C16 and higher. In addition, greater solubility is seen for dicarboxylic acids as compared to their homologous single acids:

Water Solubility Trend Analysis by Carbon Chain Length

Carbon chain length	Water solubility (mg/L)
C6, single and C8-10, di	>1000
C8-9	>100 - <1000
C10	>10 - <100
C12	>1 - <10
C14	>0.1 - <1
>=C16	<0.1 (as low as 10^{-5})

As expected, the potassium, sodium and ammonium salts exhibited higher water solubility as compared to the homologous acids, and the magnesium and calcium salts exhibited lower water solubility as compared to the homologous acids.

Water Solubility Trend Analysis by Carbon Chain Length – Salts

Carbon chain length (potassium or sodium salt)	Water solubility (mg/L)
C6 to C12	>1000
C14	>100 to <1000
C16	>10 to <100
C18	>1 to <10

Carbon chain length (ammonium salt)	Water solubility (mg/L)
C12	>100 to <1000
C18	>0.1 to < 1

Carbon chain length (magnesium, calcium salt)	Water solubility (mg/L)

C14 to C18	<0.1 (as low as 10^{-11})

Human Health

Tables 1 and 2 provide a summary of the data for mammalian endpoints as well as the read across approach for filling these endpoints.

Toxicokinetics
Short (<= 6 carbons) and medium (6-12 carbon) chain aliphatic acids are directly absorbed into blood from the intestines. Long (>12 carbon) chain aliphatic acids are absorbed in the intestine and distributed in the blood as chylomicrons. Aliphatic acids serve as a fuel for muscular contraction and general metabolism. They are consumed by mitochondria to produce ATP through beta oxidation. Fatty acid oxidation begins with activation of the molecule in the cytosol. In this reaction, a thioester bond is formed between the carboxylic group of the fatty acid and the thiol group of coenzyme A. The activated from of the fatty acid is an acyl-CoA, the exact nature of which depends on the nature of the fatty acid itself. The acyl-CoA can then cross into the mitochondria where beta-oxidation progressively shortens fatty acids two-carbons at a time as acetyl-CoA units are removed with each round of the cycle. Fatty acids that enter beta-oxidation with an even number of carbons are converted entirely to acetyl-CoA, with the last round producing two acetyl-CoA molecules from one four carbon fatty acid. The number of molecules of acetyl-CoA produced is equal to half the number of carbon atoms in the original fatty acid. For fatty acids that have an odd number of carbons, the last round of beta-oxidation with a five-carbon chain releases acetyl-CoA and the 3-carbon chain propionyl-CoA. Propionyl-CoA is converted to succinyl-CoA, an intermediate in the Kreb's cycle. Propionyl-carboxylation of propionyl-CoA as four carbons, so one of the first steps in this pathway is the carboxylation of propionyl-CoA with an input of energy from ATP. The saturation of a fatty acid has less of a bearing on the metabolism than the length of the fatty acid chain; the longer the chain, the more rounds of beta-oxidation necessary.
Acute inhalation toxicity
Single Component (sponsored substances):
The one hour LC50 for **octadecanoic acid, magnesium salt (CAS No 557-04-0)** in rats was > 2 mg/L and < 200 mg/L (no guideline specified).

Acute oral (gavage) toxicity The acute oral LD_{50} values in rats for both sponsored and supporting substances were greater than >2000 mg/kg bw (according to or similar to OECD TG 401). Clinical signs were generally associated with poor condition following administration of high doses (salivation, diarrhea, staining, piloerection and lethargy). There were no adverse effects on body weight in any study. In some studies, excess test substance and/or irritation in the gastrointestinal tract was observed at necropsy.
Single Component (sponsored substances):
In an OECD TG 401 study, a group of five rats/sex was administered **octanoic acid (CAS No 124-07-2)** at a dose of 2000 mg/kg bw. There were no deaths, clinical signs, or findings at gross necropsy. The LD50 was > 2000 mg/kg bw.
In a study conducted according to the Federal Hazardous Substance Act (FHSA), groups of five male rats were administered **decanoic acid (CAS No 334-48-5)** at doses up to 10,000 mg/kg bw. There were no deaths. There were no clinical signs observed at 464 or 1000 mg/kg bw; at 2150 mg/kg bw, transient clinical signs included wheezing, salivation, serum, blood and urine, and at 4640 and 10,000 mg/kg bw there was transient excessive salivation and diarrhea. Depression, depressed righting and placement reflexes, and unkempt fur was noted in the 10,000 mg/kg bw group. Gross necropsy findings were not reported. The LD50 was > 10,000 mg/kg bw.
In an OECD TG 401 study, a group of five rats/sex was administered **dodecanoic acid (CAS No 143-07-7)** at a dose of 5000 mg/kg bw. There were no deaths. Transient slight piloerection was observed. At necropsy, stomach mucous membrane appeared slightly reddened. The LD50 was > 5000 mg/kg bw.
In a study conducted according to the FHSA, groups of five male albino rats were administered **tetradecanoic acid (CAS No 544-63-8)** at doses up to 10,000 mg/kg bw. There were no deaths. There were no clinical signs at 464, 1000, 2150 mg/kg bw. Transient slight diarrhea and excessive salivation was observed at 4640 mg/kg bw. The majority of animals in the 10,000 mg/kg group showed slight depression, mucoid diarrhea, unkempt fur stained with diarrhea, and serum and blood discharge from the nose and eyes the first three days of dosing. There were no findings at gross necropsy. The LD50 was > 10,000 mg/kg bw.
In an OECD TG 401 study, a group of five rats/sex was administered **hexadecanoic acid (CAS No 57-10-3)** at a

dose of 5000 mg/kg bw. There was one death. Animals exhibited transient slight piloerection and reduced activity. At necropsy, animals exhibited swelling of the stomach mucous membranes. The LD50 was > 5000 mg/kg bw.

In an OECD TG 401 study, a group of five rats/sex was administered **octadecanoic acid (CAS No 57-11-4,** as a 50% suspension in DMSO) at a dose of 5000 mg/kg bw. There was one death. Animals exhibited transient piloerection, excessive salivation, and diminished activity. At necropsy, the male animal that died exhibited a stomach full of test substance; surviving animals showed remnants of test substance in the stomach with swelling of the mucous membrane. The LD50 was > 5000 mg/kg bw.

In an OECD TG 401 study, a group of five rats/sex was administered **isooctadecanoic acid (CAS No 30399-84-9)** at a dose of 2000 mg/kg bw. There were no clinical signs, deaths, or findings at necropsy. The LD50 was > 2000 mg/kg bw.

In an OECD TG 401 study, a group of five rats/sex was administered **9-octadecenoic acid, (Z)- (CAS No 112-80-1)** at a dose of 2000 mg/kg bw. There were no clinical signs, deaths, or findings at necropsy. The LD50 was > 2000 mg/kg bw.

Single Component (supporting substances):

In an OECD TG 401 study, a group of five rats/sex was administered docosanoic acid (CAS No 112-85-6) at a dose of 2000 mg/kg bw. There were no clinical signs, deaths, or findings at necropsy. The LD50 was > 2000 mg/kg bw.

Alkyl ranges and source based (sponsored substances):

In a study conducted similar to OECD TG 401, two male and two female rats were administered **fatty acids, C14-18 (CAS No 67701-02-4)** at a dose of 2000 mg/kg bw (as a 20% suspension in peanut oil;). There were no deaths, or findings at necropsy. The LD50 was > 2000 mg/kg bw.

In an OECD TG 401 study, a group of five rats/sex was administered **fatty acids, C18-22 (CAS No 90990-11-7)** (as a 50% suspension in DMSO) at a dose of 5000 mg/kg bw. There were no deaths. Animals exhibited transient piloerection and diminished activity. During necropsy, a foreign substance was found in the stomach. The mucous membranes of the stomachs appeared red and swollen. The LD50 was > 5000 mg/kg bw.

In an OECD TG 401 study, a group of five rats/sex was administered **fatty acids, C14-18 and C16-18-unsaturated (CAS No 67701-06-8)** (as a 25% suspension in water) at a dose of 5000 mg/kg bw. There were no clinical signs, deaths, or findings at necropsy. The LD50 was > 5000 mg/kg bw.

In an OECD TG 401 study, a group of five rats/sex was administered **Fatty acids, C16-18 and C18-unsaturated (CAS No 67701-08-0)** (as a 25% suspension in water) at a dose of 5000 mg/kg bw. There were no clinical signs, deaths, or findings at necropsy. The LD50 was > 5000 mg/kg bw.

Alkyl ranges and source based (supporting substances):

In a study similar to OECD TG 401, a group of five rats/sex was administered fatty acids, tall-oil (CAS No 61790-12-3) at a dose of 10,000 mg/kg bw. Transient piloerection was observed in one male and abnormal stance was observed in one male and one female. There were no other clinical signs, deaths, or findings at necropsy. The LD50 was > 10,000 mg/kg bw.

In an acute oral study (no guideline specified), a group of five rats/sex was administered fatty acids, rape-oil (CAS No 85711-54-2) (in 2% carboxymethylcellulose) at a dose of 2000 mg/kg bw. There were no clinical signs, deaths, or findings at necropsy. The LD50 was >2000 mg/kg bw.

Dicarboxylic acids (sponsored substances):

In a study conducted similar to OECD TG 401, a group of two male rats were administered **nonanedioic acid (CAS No 123-99-9)** at a dose of 5000 mg/kg bw. There were no deaths; information regarding clinical signs, effects on body weight or findings at gross necropsy was not located. The LD_{50} was > 5000 mg/kg bw.

In a study conducted similar to OECD TG 401, a group of five rats/sex was administered **Decanedioic acid (CAS No 111-20-6)** at doses up to 3200 mg/kg bw. Clinical signs of weakness and diarrhea were reported. There were no further details. The LD_{50} was 2260 mg/kg bw.

In a study conducted similar to OECD TG 401, a group of five rats/sex was administered **hexanedioic acid (CAS No 124-04-9)** (20% in corn oil) at doses up to 6310 mg/kg bw. Mortality ratios of 0/5, 2/5, 3/5, and 5/5 occurred at 3160, 3980, 5010, and 6310 mg/kg bw, respectively. Clinical signs included reduced appetite and activity. Necropsy findings on decedents included hemorrhagic lungs, discolored livers, and acute gastrointestinal inflammation; there were no findings in survivors. The LD_{50} was 5050 mg/kg bw.

Dicarboxylic acids (supporting substances):

In an acute oral (guideline not specified), a group of three or five rats/sex were administered butanedioic acid (CAS No 110-15-6) at a dose of 2000 mg/kg bw. There were no deaths, clinical signs, or findings at gross necropsy. The LD_{50} was > 2000 mg/kg bw.

In a study conducted similar to OECD TG 401, a group of five rats/sex was administered pentanedioic acid (CAS

No 110-94-1) (50% aqueous solution) at doses up to 3980 mg/kg bw. Mortality ratios were 0/5, 3/5, 3/5, and 5/5 for the 2000, 2510, 3160, and 3980 mg/kg groups, respectively. Tremors were observed in the first 2 hours. Other signs noted included salivation and diarrhea. Necropsy findings included inflammation of gastric mucosa and liver hyperemia. The LD_{50} was 2750 mg/kg bw.

In an OECD TG 401 study, a group of five rats/sex was administered octadecanedioic acid (CAS No 871-70-5) (in corn oil) at a dose of 5000 mg/kg bw. There were two deaths; clinical signs in these animals included loose stools, hypoactivity and piloerection. At necropsy, findings in the two animals that died included distended, red stomachs and gastrointestinal tracts. The gastrointestinal tracts also contained solid blockages that were likely solidified test substance. There were no deaths, clinical signs, or findings at gross necropsy in the remaining eight animals. The LD_{50} was > 5000 mg/kg bw.

Sodium and potassium salts (supporting substances):

In a study similar to OECD TG 401 study, a group of five rats/sex was administered Fatty acids, C16-18 and C18-unsaturated, sodium salts (CAS No 68424-26-0) (in carboxymethylcellulose) by gavage at a dose of 2000 mg/kg bw. There were no deaths or clinical signs. The LD_{50} was > 2000 mg/kg bw.

Magnesium and calcium salts (sponsored substances):

Groups of rats (number and sex not specified) were administered **octadecanoic acid, magnesium salt (CAS No 557-04-0)** at doses up to 1000 mg/kg bw. A test guideline was not specified. Mild diarrhea was observed in animals at the highest dose. The LD_{50} was > 10,000 mg/kg bw.

Magnesium and calcium salts (supporting substances):

In an OECD TG 401 study, a group of five rats/sex was administered 9,10-Dihydroxy-octadecanoic acid, ammonium salt (CAS No 84753-04-8) (50% in water) at a dose of 2000 mg/kg bw. There were no deaths; clinical signs were limited to severe emaciation in one animal. Findings at necropsy included fluid in the uterus in one female and evidence of cystitis (pyelonephritis), mucus in the urinary bladder, and a slight light brown discoloration of the spleen in another female. The LD_{50} was > 2000 mg/kg bw.

Acute dermal toxicity studies were not located.

Skin and eye irritation potential, with a few stated exceptions, is chain length dependent and decreases with increasing chain length (Table 2). The animal skin irritation studies (generally similar to OECD TG 404) indicate that the C6-10 aliphatic acids are severely irritating or corrosive, while the C12 aliphatic acid is irritating, and the C14-22 aliphatic acids generally are not irritating or mildly irritating. **CAS 30399-84-9**, which is a C18 methyl branched structure, is a skin irritant. The dicarboxylic acids (C4-C9) **CAS 123-99-9** and **111-20-6** and supporting CAS 110-15-6, 110-94-1, and 124-04-9) are not skin irritants. Studies in human volunteers, using up to ten sequential 24-hour occluded exposure periods, demonstrate that the C8-12 aliphatic acids are the most irritating, with the C14-18 aliphatic acids having lower irritation potential; C7 (**CAS 111-14-8**) was the only fatty acid not reported to cause an irritation response in this study. It was not possible to determine why this discrepancy occurred and **CAS 111-14-8** was considered severely irritating based on a category read across approach. Human skin irritation studies using more realistic exposures (30-minute, 1-hour or 24-hours) indicate that the aliphatic acids have sufficient, good or very good skin compatibility. Animal eye irritation studies (generally similar to OECD TG 405) indicate that among the sponsored aliphatic acids, the C8-12 aliphatic acids are irritating to the eye while the C14-22 aliphatic acids are not irritating. Eye irritation potential of the ammonium salts does not follow chain length dependence; the C18 ammonium salts are corrosive to the eyes. No sensitisation data were located.

Repeated dose toxicity studies by the oral (diet, gavage or drinking water) route (only) were located for the sponsored and supporting substances.

Repeated dose oral

Single component (Sponsored substances):

In a 90 day study (no guideline specified), groups of ten rats/sex/group were administered **9-octadecenoic acid, (Z)- (CAS No 112-80-1)** in the diet at 5, 10 and 25% (ca. 0, 3300, 6100, 14,000 mg/kg bw/day). Three animals (two controls and one mid-dose) died from the blood collection procedure. There were no clinical signs, adverse effects on body weight, urinalysis, clinical chemistry, or hematology. Food consumption among test animals was slightly lower than among the control animals. There were no significant differences in organ/body weight ratios except for kidneys, adrenal glands and brain; female animals showed a higher organ/body weight ratio than controls. In the absence of microscopic abnormalities in these organs, this effect was not considered adverse. The

NOAEL was = 25% (14,000 mg/kg bw/day).

A group of twenty male rats were administered **9,12-Octadecadienoic acid (CAS No 60-33-3)** in the diet at a dose of 1.5 % (ca. 467 - 1970 mg/kg bw/day) for 36 weeks. There were no adverse findings; the NOAEL was = 467 - 1970 mg/kg bw/day.

Single component (supporting substances):

In an OECD TG 422 study, groups of male and female rats (13/sex/group), were administered docosanoic acid, CAS No 112-85-6) by oral gavage at doses of 0, 100, 300, 1000 mg/kg/day. For males the exposure period was 42 days; for females the exposure period was from 14 days prior to mating to day 3 of lactation (minimum of 39 days of exposure). There were no deaths or changes in general condition, no changes in body weight gain or food consumption, and no adverse histopathological, hematological or biochemical effects. The NOAEL was 1000 mg/kg bw, the highest dose tested.

Alkyl ranges and source based (supporting substances):

In a study similar to OECD TG 407 study, groups of ten male and female were administered fatty acids, tall-oil, CAS No 61790-12-3 in the diet at doses of 5, 10, and 25% (approximately equivalent to 2500, 5000, and 12,500 mg/kg/day) for 90 days. Two control rats died during blood sampling. No other deaths occurred and no clinical signs were observed. Body weight and body weight gain were not affected by treatment, but food consumption was slightly decreased at 10 and 25%. No changes in hematology, clinical chemistry or urinalysis parameters occurred at any dose. At gross pathology, no treatment-related effects were noted at any dose. No consistent organ weight changes and no histopathological effects were reported at any dose. Based on these the NOEL was 5% (approximately 2,500 mg/kg/day).

Dicarboxylic acids (supporting substances):

Groups of ten rats/sex were administered butanedioic acid, CAS No 110-15-6 in drinking water at doses of 0, 0.3, 0.6, 1.25, 2.5, 5, 10% (0, 240, 480, 1000, 2000, 4000, 8000 mg/kg bw/day) for 13 weeks. A guideline was not specified. Severe suppression of body weight gain occurred in rats in the 10% group, and all of the rats died during the first four weeks of exposure. There were no other deaths. Suppression of body weight gain was observed at 2.5 and 5%. Drinking water consumption was reduced in all exposure groups. No dose-related changes were observed in the hematology and biochemistry. There were no histopathological findings in surviving rats. On the basis of body weight depression, the maximum tolerated dose of monosodium succinate was determined to be approximately 2-2.5% (1700-2100 mg/kg bw/day) when given in the drinking water.

In a study similar to OECD TG 408, groups of 15 rats/sex/dose were fed 0, 0.5, 1.0 or 2.0% (0, 400, 800 and 1200 mg/kg bw/day) pentanedioic acid, CAS No 110-94-1 in the diet for 90 days. There were no deaths. No effects were observed on food consumption, hematology, clinical chemistry, urinalysis, organ weights or histopathology. Based on reduced body weight gains, the NOAEL is 800 mg/kg bw. Twenty rats/group were fed 0, 0.1, 1.0, 3.0, 5.0% hexanedioic acid, CAS No 124-04-9 in diet (0, 47, 1500, 2700 mg/kg bw/day); the females were fed either 0% (10 animals) or 1.0% (19 animals; 63 mg/kg bw) for 2 years. Body weight gains for the males were reduced in the 3 and 5% dose groups and food consumption was lower in the 5% dose group; these effects were not considered adverse. There were no effects on mortality, clinical signs, gross pathology, organ weights or histopathology. There were no effects on mortality, clinical signs, weight gains, food consumption, organ weights, gross pathology or histopathology for the female rats. The NOAEL is 2700 mg/kg bw/day (males) and 63 mg/kg bw (females), the highest doses tested.

In an OECD TG 407, groups of male and female rats (5/sex/dose) were administered octadecanedioic acid, CAS No 871-70-5 via oral gavage to 0 or 1000 mg/kg bw/day of the test substance daily for 28 days. No effects were observed on mortality, clinical signs, body weights, food consumption, or organ weights. No toxicologically relevant effects were observed on haematology or clinical chemistry. The NOAEL is = 1000 mg/kg bw/day.

In an OECD TG 422 study groups of male and female rats were administered dodecanedioic acid, CAS No 693-23-2 at doses of 0, 100, 500 or 1000 mg/kg bw by oral gavage. The NOAEL for systemic toxicity was 1000 mg/kg bw (the highest dose tested; limit dose) for both male and female animals.

Magnesium and calcium salts (Sponsored substances):

In a study conducted similar to OECD TG 408, groups of twenty rats/sex/group were administered **octadecanoic acid, magnesium salt (CAS No 557-04-0)** in the diet at 0, 5, 10, 20% for 90 days (4000, 8000, 16,000 mg/kg bw/day). Four males in the 20% group died in the first 8 weeks. Necropsy revealed the presence stone formation in the lower urinary pathways which likely accounted for these deaths. In the 20% group, weight gain (males) was significantly decreased in the first 8 weeks of dosing; there was also a 33% reduction in food consumption (males and females). The amount of utilizable energy in the diet decreased as the amount of test substance increased due to the relative poor absorption of the material (15-20% absorption at the 20% dosage level). This might explain the depletion of glycogen and decreased liver weight. There was a reduction in packed cell volume in the 20% group

after 12 weeks and males from the 20% group exhibited a decrease in liver glycogen. The kidney to bodyweight ratio was significantly reduced in all dosage groups for the female animals, and in the 10% group for the male animals. The liver to body weight ratio was significantly reduced in all dosage groups for the male animals, and in the 20% group for the females. The reduction in the liver to body weight ratios are likely due to the reduced food intake of the animals (33% reduction in the 20% group). The high magnesium content of the diet containing 20% magnesium stearate is likely to be the cause of the stone formation and changes in the urinary tract. Animals from the 20% group exhibited a deposition of iron in the kidney and liver (both sexes). The NOAEL is 5% in the diet, corresponding to 4000 mg/kg bw/day.

Repeated dose oral (gavage or diet) exposure to the sponsored or supporting aliphatic acids did not result in systemic toxicity with NOAELs greater than the limit dose of 1000 mg/kg bw (similar to OCED TG 407, 408 or 422). Similar results are expected for all of the category members.

Mutagenicity
The sponsored and supporting aliphatic acids are not mutagenic or clastogenic in vitro and the supporting aliphatic acids are not mutagenic or clastogenic in vitro or in vivo. Studies were similar to OECD TG 471 and 473. One exception to these results was the positive finding in an in vitro transformation assay with BALB/3T3 cells exposed to CAS 110-94-1 in the presence and absence of metabolic activation. As the only single positive result in this category, the weight of evidence indicates that members of the aliphatic acids category are not anticipated to be genotoxic.

In vitro Studies - Gene mutation
Single component (Sponsored substances):
In an OECD TG, *S. typhimurium* TA 98, TA 100, TA 1535, and TA 1537 were exposed to **hexanoic acid (CAS No 142-62-1)** at concentrations up to 800 ug/plate (cytotoxic >= 800 ug/plate) in the presence and absence of metabolic activation (Aroclor 1254 induced rat liver S-9 mix). Positive, negative and solvent controls were included and valid. The test substance was not mutagenic.
In an OECD TG 471, *S. typhimurium* TA 97, TA 98, TA 100, TA 1535, and TA 1537 were exposed to **heptanoic acid (CAS No 111-14-8)** at concentrations up to 6666 ug/plate (up to 1666 ug/plate for TA 97) in the presence and absence of metabolic activation (rats and hamsters induced with 10% or 30% Aroclor). Positive and solvent controls were included. Solvent controls were valid; validity data were not located for positive controls. The test substance was not mutagenic.
In a study conducted similar to OECD TG 471, *Salmonella (S.) typhimurium* TA 98, TA 100, TA 1535, and TA 1537 were exposed to **octanoic acid (CAS No 124-07-2)** at concentrations up to 1250 ug/plate in the presence and absence of metabolic activation (Aroclor 1254 induced rat liver S-9 mix). There was no information regarding positive, negative and solvent controls. The test substance was not mutagenic.
In an OECD TG 471, *S. typhimurium* TA 98, TA 100, TA 1535, and TA 1537 were exposed to **isooctadecanoic acid (CAS No 30399-84-9)** at concentrations up to 5000 ug/plate in the presence and absence of metabolic activation (Aroclor 1254 induced rat liver S-9 mix). Positive, negative and solvent controls were included and valid. The test substance was not mutagenic.
In an Ames test (no guideline specified), *S. typhimurium* TA 98, TA 100, TA 1535, TA 1537 and TA 1538 were exposed to **12-hydroxy-octadecanoic acid (CAS No 106-14-9)** at concentrations up to 2500 ug/plate in the presence and absence of metabolic activation (Aroclor 1254 induced rat liver S-9 mix). Positive and negative controls were included but results of the controls were not located. The test substance was not mutagenic.
In a mouse lymphoma assay, mouse lymphoma L5178Y cells were exposed to **12-hydroxy-octadecanoic acid (CAS No 106-14-9)** at concentrations up to 250 ug/plate in the absence of metabolic activation and up to 100 ug/plate in the presence of metabolic activation (Aroclor-induced rat liver S-9). Positive and solvent controls were included and valid. The test substance was not mutagenic.
In a Bacterial Reverse Mutation Assay (no guideline specified), *S. typhimurium* TA 98, TA 100, TA 1535, and TA 1537 were exposed to **9-Octadecenoic acid, (Z)- (CAS No 112-80-1)** at concentrations up to 10,000 ug/plate in the presence and absence of metabolic activation (Aroclor 1254 induced rat or hamster liver S-9 mix). Positive, negative and solvent controls were included but results of the controls were not located. The test substance was not mutagenic.
In a study similar to OECD TG 471, *S. typhimurium* TA 98, TA 100, TA 1535, TA 1537 and/or TA 97 were exposed to **9,12-Octadecadienoic acid (CAS No 60-33-3)** (concentrations not specified) in the presence and absence of metabolic activation (Aroclor 1254 induced rat liver S-9 mix; Zeiger et al. , 1987). Positive and solvent

controls were included and valid. The test substance was not mutagenic.

Single component (supporting substances):

In an OECD TG 471, *S. typhimurium* TA 100, TA 1535, TA 98, TA 1537 and *E. coli* WP2 uvrA were exposed to docosanoic acid (CAS No 112-85-6) at concentrations up to 5000 ug/plate in the presence and absence of metabolic activation (liver, induced with phenobarbital and 5,6-benzoflavone). Negative and solvent controls were included and valid; there was no data located regarding positive controls. The test substance was not mutagenic.

Alkyl ranges and source based (supporting substances):

In a study similar to OECD TG 471, *S. typhimurium* TA 98, TA 100, TA 1535, TA 1537 and/or TA 97 were exposed to fatty acids, tall-oil (CAS No 61790-12-3) at concentrations up to 10,000 ug/plate in the presence and absence of metabolic activation (Aroclor 1254 induced rat liver S-9 mix). Positive controls were included but results of the controls were not located. The test substance was not mutagenic.

Dicarboxylic acids (Sponsored substances):

In an OECD TG 471, *S. typhimurium* TA 98, TA 100, TA 1535, TA 1537, TA 1538 were exposed to **Decanedioic acid (CAS No 111-20-6)** at concentrations up to 5000 ug/plate in the presence and absence of metabolic activation (Aroclor 1254 induced rat liver S-9 mix). Positive, negative and solvent controls were included but results of the controls were not located. The test substance was not mutagenic.

Dicarboxylic acids (Supporting substances):

In an Ames test, *S. typhimurium* TA 92, TA 1535, TA 100, TA 1537, TA 94, and TA 98 were exposed to butanedioic acid (CAS No 110-15-6) at concentrations up to 5000 ug/plate in the presence and absence of metabolic activation (biphenyl KC-400-treated rat liver S-9). The test substance was not mutagenic.

In an Ames test, *S. typhimurium* TA 98, TA 100, TA 1535, TA 1537, and TA 1538 were exposed to pentanedioic acid (CAS No 110-94-1) at concentrations up to 5000 ug/plate in the presence and absence of metabolic activation. Positive and negative controls were included but results of the controls were not located. The test substance was not mutagenic.

In a mouse lymphoma assay (conducted according to Clive and Spector, 1975), mouse lymphoma L5178Y cells were exposed to pentanedioic acid (CAS No 110-94-1) at concentrations of 156 - 8295 ug/ml in the presence of metabolic activation (Aroclor-induced rat liver S-9). Concurrent negative and positive controls were run. Positive and solvent controls were included and but results not located. The test substance was not mutagenic.

In an in vitro transformation assay, BALB/3T3 cells were exposed to pentanedioic acid (CAS No 110-94-1) at concentrations up 12.5 mg/mL in the absence of metabolic activation (rat liver microsomes) and up to 26.3 mg/mL in the presence of metabolic activation. Concurrent negative and positive controls were run. The substance induced a significant, dose-related number of transformed foci under non-activation (3.3-12.5 mg/mL) and activation (16.8 and 21 mg/mL) conditions. Therefore, the substance was considered to be active in the BALB/3T3 in vitro transformation assay in the absence and presence of an exogenous metabolic activation system.

In an OECD TG 471, *S. typhimurium* TA 98, TA 100, TA 102, TA 1535, and TA 1537 were exposed to octadecanedioic acid (CAS No 871-70-5) at concentrations up to 5000 ug/plate in the presence and absence of metabolic activation. Positive, negative and solvent controls were included and valid. The test substance was not mutagenic.

In an Ames test (no guideline specified), *S. typhimurium* TA 98, TA 100, TA 1535, and TA 1537 were exposed to dodecanedioic acid (CAS No 693-23-2) at concentrations up to 5000 ug/plate in the presence and absence of metabolic activation. There was no data located regarding controls. The test substance was not mutagenic.

In an in vitro Bacterial Reverse Mutation Assay (Ames et al. (1975), *S. typhimurium* TA 98, TA 100, TA 1535, TA 1537, TA 1538 and *Escherichia coli* strain WP2 were exposed to hexanedioic acid (CAS No 124-04-9) at concentrations up to 10,000 ug/plate in the presence and absence of metabolic activation (Aroclor®-induced rat liver S-9). Positive controls were included and valid. The test substance was not mutagenic.

In an OECD TG 471 (Bacterial Reverse Mutation Assay), *S. typhimurium* TA 98, TA 100, TA 102, TA 1535, and TA 1537 were exposed to octadecanedioic acid (CAS No 871-70-5) at concentrations up to 5000 ug/plate in the presence and absence of metabolic. Positive, negative and solvent controls were included and valid. The test substance was not mutagenic.

Magnesium and calcium salts (sponsored substances):

In a Bacterial Reverse Mutation Assay (no guideline specified), *S. typhimurium* TA 1535, TA 1537 and TA 1538 and *Saccharomyces cerevisae* D4 were exposed to **octadecanoic acid, magnesium salt (CAS No 557-04-0)** (concentrations not specified) in the presence and absence of metabolic activation (rat, mouse and monkey liver and lung; Busch, 1982). Further details were not located. The test substance was not mutagenic.

Ammonium salts (Supporting substances):

In an OECD TG 471, *S. typhimurium* TA 98, TA 100, TA 1535, TA 1537 and TA 1538 were exposed to 9,10-Dihydroxy-octadecanoic acid, ammonium salt (CAS No 84753-04-8) at concentrations up to 5000 ug/plate in the presence and absence of metabolic activation (Aroclor 1254 induced rat liver S-9 mix). Positive controls were included but results of the controls were not located. The test substance was not mutagenic.

In vitro studies - Chromosome aberration

Single component (Sponsored substances):

In a study similar to OECD TG 473, Chinese Hamster Ovary (CHO) cells were exposed to **12-hydroxy-octadecanoic acid (CAS No 106-14-9)** at concentrations up to 213 ug/ml in the presence and absence of metabolic activation (rat liver S-9 induced with Aroclor 1254). Solvent and positive controls fulfilled the requirements for a valid study. The test substance did not induce chromosomal aberrations in this study.

Single component (Supporting substances):

In an OECD TG 473 study, Chinese hamster lung fibroblasts (V79) were exposed to docosanoic acid (CAS No 112-85-6) in the presence and absence of metabolic activation (Rat liver, induced with phenobarbital and 5,6-benzoflavone), The concentrations for the 24 hour exposure were 0, 350, 700, 1400, 2800 µg/ml; for the 48 hour exposure the concentrations were 0, 288, 575, 1150, 2300 µg/ml. For the short term exposure the concentrations were 0, 875, 1750, 3500 µg/ml and for the long term exposure the concentrations were 0, 875, 1750, 3500 µg/ml. Positive and negative controls were included and valid. There were no further details. The test substance was not clastogenic.

Dicarboxylic acids (Supporting substances):

In a chromosome aberration test (guideline not specified), Chinese hamster fibroblasts were exposed to butanedioic acid, CAS No 110-15-6 at concentrations up to 1.0 mg/mL in the absence of metabolic activation. The cells were exposed to the test substance at three different doses for 24 and 48 hours. Solvent and negative controls were included but results of the controls were not located. The test substance did not induce chromosomal aberrations in this study.

In an in vitro cytogenetic study in anaphase cells (guideline not specified), human embryonic lung cell cultures (WI-38) were exposed to hexanedioic acid, CAS No 124-04-9 in the absence of metabolic activation at concentrations of 0, 2, 20 and 200 ug/mL (USFDA, 1974). Positive and negative controls were included but results of the controls were not located. The test substance did not induce any of the analyzed aberrations (bridges, pseudochiasmata, multipolar cells, and acentric fragments).

In an OECD TG 473 study, V79 cells were exposed to 1,18-octadecanedioic acid (CAS No 871-70-5) in the presence and absence of metabolic activation. In experiment I, concentrations were tested up to 50 µg/ml without metabolic activation and up to 52.5 µg/mL with metabolic activation. In experiment II, concentrations were tested up to 50 µg/mL without metabolic activation and up to 31.5 µg/mL with metabolic activation. Positive, negative and solvent controls were included and valid. The test substance was not clastogenic.

In vivo studies

Dicarboxylic acids (Supporting substances):

In an in vivo mouse micronucleus study (guideline not specified), groups of four mice/sex were administered pentanedioic acid, CAS No 110-94-1 by intraperitoneal injection 800 mg/kg bw and sacrificed at 30 or 48 hours. Two additional groups of animals were given two injections of 800 mg/kg bw at 0 and 24 hours and sacrificed at 48 or 72 hours, respectively, after the first dose. Similar groups, serving as the positive and negative control, were evaluated concurrently (results from controls not located). The test substance did not produce a statistically significant increase in micronuclei in any of the treated groups, and was determined to be negative in this assay.

In an in vivo Rat Cytogenetic Chromosomal Aberration Assay (guideline not specified), groups of male rats/group [(nine negative controls and five positive controls); five per dose group for the subacute study (three negative controls)] were administered hexanedioic acid, CAS No 124-04-9 by oral gavage. In the acute tests, animals were given a single dose of the test substance (Test I: 0, 3.75, 37.5, 375 mg/kg bw; Test II: 0, 5000 mg/kg bw) and killed 6, 24, or 48 hours after administration. For the subacute tests, animals were given 5 doses (Test I: 0, 3.75, 37.5, 375 mg/kg bw; Test II: 0, 2500 mg/kg bw) 24 hours apart and killed six hours after the last dose. Positive and negative controls were included and valid. The test substance was not mutagenic.

In an in vivo dominant lethal assay, groups of ten male rats were administered hexanedioic acid, CAS No 124-04-9 by gavage for five days at doses of 3.75-375 mg/kg (experiment I); 5000 mg/kg (experiment II) or 2500 mg/kg (experiment II). Following treatment, the males were sequentially mated to two females per week for eight weeks. Females were sacrificed 14 days after separating from the male, and at necropsy the uterus was examined for early deaths, late fetal deaths, and total implantations. The fertility index, preimplantation loss, and lethal effects on the embryos were determined. Positive and negative controls were included and valid. There was no effect of

treatment and the test substance was concluded to not induce dominant lethal mutations.

Carcinogenicity
No data were located for carcinogenicity of the sponsored substances.

Reproductive toxicity
No effects on fertility or on reproductive organs (similar to OECD TG 408 or 422), or developmental effects (similar to OECD TG 422 or 416) were observed in studies on the sponsored or supporting aliphatic acids and the NOAELs correspond to the maximum dose tested. The weight of evidence supports the lack of reproductive and developmental toxicity potential of the aliphatic acids category.

Effects on Fertility/Reproductive organs
Single component (Sponsored substances):
In a 90 day study (no guideline specified), groups of ten rats/sex/group were administered **9-Octadecenoic acid, (Z)- (CAS No 112-80-1)** in the diet at 0, 3300, 6100, 14,000 mg/kg bw/day. There were no effects on gonads weights, and no gross or histopathological findings for testes, seminal vesicle, ovary, uterus, or prostate. The NOAEL for reproductive effects was 14,000 mg/kg bw, the highest dose tested.
A group of twenty male 344 rats were administered **9,12-octadecadienoic acid (CAS No 60-33-3)** in the diet at a dose of ca. 467 - 1970 mg/kg bw/day for 36 weeks. There were no effects on testes weights, no findings at gross necropsy or histopathological findings in the testes; the NOAEL for male reproductive effects was = 467 - 1970 mg/kg bw/day, the highest dose tested.
Single component (Supporting substances):
In an OECD TG 422 study, rats (13/sex/dose) were exposed to 0, 100, 300, or 1000 mg/kg bw/day of docosanoic acid, CAS No 112-85-6 via oral gavage. For males the exposure period was 42 days; for females the exposure period was from 14 days prior to mating to day 3 of lactation (minimum of 39 days of exposure). There were no effects on gonadal function, mating behaviour, conception, development of the conceptus or parturition. The NOAEL for reproductive toxicity is >= 1000 mg/kg bw/day, the highest dose tested.
Alkyl ranges and source based (Supporting substances):
In a two generation study (similar to OECD TG 416; the initial treatment period was decreased to three weeks versus ten weeks), groups of rats (30 females/15 males/dose) were administered 0, 5 or 10% fatty acids, tall-oil, CAS No 61790-12-3 in the diet, (equivalent to approximately 0, 2500 or 5000 mg/kg bw/day). The parental (F0) generation began treatment at 80 days of age and were mated at 100 days of age. Treatment continued through the weaning of the first generation (F1). After weaning, 20 F1 males and 20 F1 females per group were maintained on the parental diet. At 100 days of age, these rats were mated and allowed to deliver pups (F2). Treatment did not affect the number of live born or stillborn F1 litters and pups, or F1 weaning weight. No treatment-related changes in fertility, viability, lactation, or gestation indices were measured. Hematology, clinical chemistry and urinalysis parameters were unchanged, and gross and microscopic pathology revealed no treatment-related effects. The NOAEL for reproductive toxicity is >= ca. 5000 mg/kg bw/day for rats exposed for two generations.
Dicarboxylic acids (Supporting substances):
Male rats (20/dose) were fed 0, 0.1, 1.0, 3.0 or 5.0% diet (0, 47, 1500, 2700 mg/kg bw/day) hexanedioic acid, CAS No 124-04-9 in the diet and females were fed either 0% (10 animals) or 1.0% (19 animals; 63 mg/kg bw) for 2 years. There were no effects on testes weight. There were no histopathological findings for testes, ovaries or uterus. The NOAEL for effects on reproductive endpoints was 2700 mg/kg bw/day (males) and 63 mg/kg bw (females), the highest doses tested.
In an OECD TG 422 study, groups of twelve rats/dose were exposed to 0, 100, 500, or 1000 mg/kg bw/day of dodecanedioic acid, CAS No 693-23-2 by oral gavage. There were no effects on reproductive endpoints (mating index, fertility index, gestation index, pups born alive, viability index, and litter survival). The NOAEL for reproductive toxicity is >= 1000 mg/kg bw/day, the highest dose tested.
Magnesium and calcium salts (Sponsored substances):
In a study conducted similar to OECD TG 408, groups of twenty rats/sex/group were administered the octadecanoic acid, magnesium salt (CAS No 557-04-0) in the diet at 4000, 8000, 16,000 mg/kg bw/day for 90 days. There were no effects on reproductive organ weight or at gross necropsy for the testes and ovaries, and no histopathological findings for the testes, ovaries or uterus. The NOAEL for reproductive effects was 4000 mg/kg bw, the highest dose tested.

Developmental Toxicity

Single component (Sponsored substances):
In a study following the Chernoff/Kavlock Developmental Toxicity Screen, groups of female mice (26-30/dose) were treated via oral gavage on gestation days 8-12 with 10,000 mg/kg bw/day of **9,12-octadecadienoic acid (CAS No 60-33-3)**. There were no effects on number of litters, number of resorptions, number of pups/litter, number of live and dead births, postnatal survival rates, pup weights at days 1 and 3 or external abnormalities among dead pups. The NOEL for developmental toxicity is >= 10,000 mg/kg bw/day for mice with exposure on gestation days 8-12.

Single component (Supporting substances):
In an OECD TG 422 study, groups of rats (13/sex/dose) were exposed to 0, 100, 300, or 1000 mg/kg bw/day of docosanoic acid, CAS No 112-85-6 the test substance via oral gavage. For males, the exposure period was 42 days; for females from 14 days prior to mating to day 3 of lactation (minimum of 39 days). The number of live and stillborn pups was noted as well as the number that died postpartum. On day 4 of lactation, pups were necropsied. There were no effects on developmental parameters. The NOAEL for developmental toxicity is >= 1000 mg/kg bw/day, the highest dose tested.

Alkyl ranges and source based (Supporting substances):
In a two generation study (similar to OECD TG 416; the initial treatment period was decreased to three weeks versus ten weeks), groups of rats (30 females/15 males/dose) were administered 0, 5 or 10% of fatty acids, tall-oil, CAS No 61790-12-3 in the diet, (equivalent to approximately 0, 2500 or 5000 mg/kg bw/day). The parental (F0) generation began treatment at 80 days of age and were mated at 100 days of age. Treatment continued through the weaning of the first generation (F1). After weaning, 20 F1 males and 20 F1 females per group were maintained on the parental diet. At 100 days of age, these rats were mated and allowed to deliver pups (F2). Treatment did not affect the number of live born or stillborn F1 litters and pups, or F1 weaning weight. No treatment-related changes in fertility, viability, lactation, or gestation indices were measured. Hematology, clinical chemistry and urinalysis parameters were unchanged, and gross and microscopic pathology revealed no treatment-related effects. The NOAEL for developmental toxicity is >= ca. 5000 mg/kg bw/day for rats exposed for two generations.

Dicarboxylic acids (Supporting substances):
In a standard developmental study (guideline not specified), groups of 25 female rats were exposed to 0, 125, 400 or 1300 mg/kg bw of pentadecanoic acid, CAS No 110-94-1 via oral gavage on gestation days 6-15 with caesarean section on day 20. There were two deaths at 1300 mg/kg bw. Mean body weight gains were decreased only in the 1300 mg/kg bw dose group (during the dosing period); mean body weight gains post-dosing (gestation days 15-20) were normal compared to control. Clinical signs observed at 1300 mg/kg bw included salivation, rales, nasal discharge, slight inactivity, labored breathing, decreased body temperature, soft stools, and staining around the mouth, nares, and anogenital area. At 400 mg/kg bw, clinical signs included salivation, rales, and nasal discharge. No adverse effects were observed on body weight, general appearance, or behavior of rats at 125 mg/kg bw. The NOAEL for maternal toxicity is 125 mg/kg bw/day for rats exposed on gestation days 6-15. No adverse effects on pregnancy or no teratogenic effects were observed. The NOAEL for developmental toxicity is >= 1300 mg/kg bw/day for rats exposed on gestation days 6-15.

Groups of female rats (24-25/dose) were exposed via oral gavage to 0, 2.9, 13, 62 and 288 mg/kg bw of hexanedioic acid, CAS No 124-04-9 on gestation days 6-15 with caesarean section on day 20 (guideline not specified). No adverse effects on pregnancy, and no embryotoxic or teratogenic effects were observed. The NOAEL for maternal and developmental toxicity is >= 288 mg/kg bw/day, the highest dose tested, for rats exposed on gestation days 6-15.

In an OECD TG 422 study, rats were exposed to 0, 100, 500, or 1000 mg/kg bw/day of dodecanedioic acid, CAS No 693-23-2. After 14 days of dosing, rats were mated within the treatment groups and allowed to produce litters. Dosing continued through mating, gestation and lactation until day 54. There were no effects on developmental parameters. The NOAEL for parental toxicity and developmental toxicity is >= 1000 mg/kg bw/day, the highest dose tested.

The Aliphatic Acids category members possess properties indicating a hazard for human health (severe skin irritation/corrosion for C6-C10 [except for the dicarboxylic acids which are not irritating], irritating to the skin for C12 and methyl branched C18, irritating to the eye for C8-C12 and dicarboxylic acids (based on read-across to supporting substances). Adequate screening-level data are available to characterize the hazard to human health for the purposes of the OECD Cooperative Chemicals Assessment Programme.

Environment

The aliphatic acids of this category are of similar very weak acid strength (approximately pKa 5), i.e., partially dissociate in aqueous solution; the salts of the aliphatic acids are highly dissociated in water solution such that the anion is the same for homologous salts and acids.

OECD TG 111 studies have not been conducted for the aliphatic acids. Hydrolysis is not an important fate path in the environment due to the fact that the substances lack hydrolysable functional groups. Aliphatic acids are hydrolytically stable in aqueous solutions.

The aliphatic acids are subject to photodegradation in air. Modeled photodegradation rates (half-lives) using AopWin v1.92 (EPI Suite v4.10) are based on the hydroxyl radical reaction at 25ºC (12-hr day; 1.5E6 OH/cm^3). Estimated half-lives generally increase with decreasing chain length and range from 0.6 hours (**9,12,15-Octadecatrienoic acid, (Z,Z,Z), CAS No. 463-40-1**, C18) to 17.5 hours (**Octanoic acid, sodium salt, CAS No. 1984-06-1**, C8). Level III fugacity modelling using EPI Suite v4.10 indicates that the aliphatic acids will distribute primarily to soil and water, with lesser amounts to air and sediment. With increasing chain length, the percent distributions to soil and sediment generally increase and the percent distributions to water and air generally decrease.

Biodegradation studies or model estimations for single and multi-component aliphatic acids generally confirm that the extent of biodegradation observed in 28 days meets the ready biodegradability criterion (>60%). In some cases, insufficient sampling points were included in the tests to determine whether or not the 10-day window was met and thus are insufficient to demonstrate ready biodegradability. When the 10-day window was not met or less than 60% biodegradation was observed in 28 days, it is likely that the aliphatic acids tested were not fully in solution. **Fatty acids, C14-22, CAS 68424-37-3** was the only sponsored substance that did not reach 60% biodegradation in 28 days, and is likely due to its poor water solubility. Modeling results for the magnesium (**Octadecanoic acid, magnesium salt; CAS 557-04-0**) and calcium (**Hexadecanoic acid, calcium salt, CAS 542-42-7**) salts indicate these substances are not readily biodegradable, most likely due to the expected low water solubility of the substances. However, the BKH Environmental data review of soaps states that the available data indicate all fatty acid salt chain lengths up to and including C18 can be metabolised under aerobic conditions and can be considered to be biodegradable. Biodegradability did not appear to be influenced by even or odd chain length, degree of saturation or unsaturation or branching. For example, odd/even chain length: C8 and C9 are readily biodegradable; Saturation/unsaturation: C18 (saturated) and C18 (di-unsaturated) are biodegradable, while C18 (mono-unsaturated) are readily biodegradable; branching or hydroxylation: the C18 hydroxylated substance was readily biodegradable and the C18 methyl branched substance was biodegradable. The aliphatic acids also undergo biodegradation under anaerobic conditions.

Estimated bioconcentration factor values are calculated using EPI Suite v4.10. The aliphatic acids have BCF values less than 100, indicating a low potential for bioaccumulation.

Summary of modeled BCF

Substance	Modeled BCF
Single Component	3.16 – 56.2
Alkyl Ranges and Source Based	3.16 – 56.2
Dicarboxylic acids	3.16
Sodium and potassium salts	3.16 – 56.2
Magnesium and calcium salts	3.38-72
Ammonium salts	3.16-70.8

The following acute toxicity test results have been determined for aquatic species (key studies only):

Substance	**Species**	**Effect level**	**Study Design**
	Fish	**LC_{50} (mg/L), 96 hr**	
Single component			
Sponsored substances			
Hexanoic acid; 142-62-1	*Pimephales promelas*	320 (measured)	No guideline specified, flow through
Nonanoic acid; 112-05-0	*Pimephales promelas*	104 (measured)	No guideline specified, flow

			through
Decanoic acid; 334-48-5	*Oryzias latipes*	20 (freshwater, nominal, 48 hr) 31 (seawater, measured, 48 hr)	No guideline specified, semi-static
Dodecanoic acid; 143-07-7	*Danio rerio*	150 (nominal) exceeds water solubility	OECD TG 203, static
Tetradecanoic acid; 544-63-8	*Leuciscus idus*	>100 - <300 (nominal) exceeds water solubility	Similar to OECD TG 203, semi-static
Hexadecanoic acid; 57-10-3	*Danio rerio*	>1000 (nominal) exceeds water solubility	Similar to OECD TG 203, semi-static
Octadecanoic acid; 57-11-4	*Danio rerio*	>1000 (nominal) exceeds water solubility	OECD TG 203, static
Isooctadecanoic acid; 30399-84-9	*Cyprinus carpio*	13.4 (nominal, 48 hr) exceeds expected water solubility	Evaluation of water-endangering materials, determination of the acute fish toxicity, Ad-hoc-working group 1, static
9-Octadecenoic acid, (Z)-; 112-80-1	*Oncorhynchus mykiss*	>56 (nominal; highest concentration tested) exceeds expected water solubility	No guideline specified, semi-static
Supporting substances			
9,10-Dihydroxy-octadecanoic acid; 120-87-6	*Danio rerio*	> 10000 (nominal) exceeds expected water solubility	EU 92/69/EWG/ Semi-static
Alkyl ranges and source based			
Sponsored substances			
Fatty acids, C6-12; 67762-36-1	*Danio rerio*	38 (nominal) exceeds expected water solubility of some components	OECD TG 203, semi-static
Fatty acids, C16-18; 67701-03-5	*Leuciscus idus*	>1000 (nominal; 48 hr) exceeds expected water solubility	Similar to OECD TG 203, static
Fatty acids, C18-22; 90990-11-7	*Danio rerio*	>100 (nominal) exceeds expected water solubility	Similar to OECD TG 203, semi-static
Fatty acids, C14-18 and C16-18-unsaturated; 67701-06-8	*Danio rerio*	>1000 (nominal) exceeds expected water solubility	Similar to OECD TG 203, semi-static
Fatty acids, C16-18 and C18-unsaturated; 67701-08-0	*Danio rerio*	300 (nominal) exceeds expected water solubility	Similar to OECD TG 203, semi-static
Fatty acids, tallow; 61790-37-2	*Cyprinus carpio*	Not toxic at limit of solubility	OECD TG 203, static
Supporting substances			
Fatty acids, sunflower, conjugated; 68953-27-5	*Danio rerio*	110 (nominal) exceeds expected water solubility	Similar to OECD TG203/semi-static
Dicarboxylic acids			
Sponsored substances			
Nonanedioic acid; 123-99-9	*Leuciscus idus*	310 (nominal; 48 hr)	Similar to OECD TG 203, static
Decanedioic acid; 111-20-6	*Danio rerio*	>9.67 (measured; highest concentration tested)	OECD TG 203, static
Supporting substances			
Hexanedioic acid; 124-04-9	*Pimephales promelas*	97 (nominal)	No guideline specified, static
Octadecanedioic acid; 871-70-5	*Danio rerio*	>100 (nominal; exceeds expected water solubility); WAF = 0.14-0.22	OECD TG 203, semi-static
Sodium and potassium salts			
Sponsored substances			
Octanoic acid, sodium salt; 1984-06-1	*Oryzias latipes*	310 (nominal)	No guideline specified, semi-static
Decanoic acid, sodium salt; 1002-62-6	*Oryzias latipes*	54 (nominal; WAF)	No guideline specified, semi-static
Dodecanoic acid, sodium salt; 629-25-4	*Oryzias latipes*	11 (nominal; WAF)	No guideline specified, semi-static
Tetradecanoic acid, sodium salt; 822-12-8	*Oryzias latipes*	118 (nominal)	No guideline specified, semi-static
Hexadecanoic acid, sodium salt; 408-35-5	*Oryzias latipes*	150 (nominal) exceeds expected water solubility	No guideline specified, semi-static
Octadecanoic acid, sodium salt; 822-16-2	*Oryzias latipes*	125 (nominal) exceeds expected water solubility	No guideline specified, semi-static
9-Octadecenoic acid, (Z)-, potassium salt; 143-18-0	*Lepomis macrochirus*	23 (not specified) exceeds expected water solubility	No guideline specified, static

Supporting substances			
Fatty acids, C16-18 and C18-unsaturated, sodium salts; 68424-26-0	*Danio rerio*	54 (nominal) exceeds expected water solubility	Similar to OECD TG 203/semi-static
	Aquatic invertebrate	**EC_{50} (mg/L), 48 hr**	
Single component			
Sponsored substances			
Hexanoic acid; 142-62-1	*Hyale plumulosa*	235 (measured, 48 hr, saltwater)	No guideline specified, no further details
Octanoic acid; 124-07-2	*Hyale plumosa*	128 (measured)	No guideline specified, semi-static
Decanoic acid; 334-48-5	*Hyale plumosa*	41 (measured; Water Accommodated Fraction (WAF)	No guideline specified, semi-static
Dodecanoic acid; 143-07-7	*Hyale plumosa*	>5.6 (nominal, WAF, limit of solubility) exceeds water solubility	No guideline specified, semi-static
Tetradecanoic acid; 544-63-8	*Hyale plumosa*	No mortality at saturation in seawater	No guideline specified, semi-static
9-Octadecenoic acid, (Z)-; 112-80-1	*Daphnia magna*	EC_0 >=32 (nominal; highest concentration tested; WAF, water hardness of 54 or 215 mg/L) exceeds expected water solubility	EC Guideline C2, static
9,12-Octadecadienoic acid; 60-33-3	*Daphnia magna*	55 (nominal, WAF) exceeds expected water solubility	EU 92/69/EWG, static
Alkyl ranges and source based			
Sponsored substances			
Fatty acids, tallow, hydrogenated; 61790-38-3	*Daphnia magna*	EC_0 >100 (nominal) exceeds expected water solubility	Static Acute Freshwater Invertebrate Toxicity Study of P1943.01, R.D. Vashon, 2-28-85, based on "Method for acute toxicity tests with fish, macroinvertebrates and amphibians," (US EPA 1975), static
Supporting substances			
Fatty acids, C16-22 and C18-22 unsaturated; 95912-82-6	*Daphnia magna*	0.695 (WAF, measured)	EU 92/69/EWG, static
Dicarboxylic acids			
Sponsored substances			
Decanedioic acid; 111-20-6	*Daphnia magna*	>11.6 (nominal)	OECD TG 202, static
Supporting substances			
Butanedioic acid; 110-15-6	*Daphnia*	374.2 (nominal, 48 hrs)	EPA (1975), static
Hexanedioic acid; 124-04-9	*Daphnia magna*	Ec0 = 62.5, EC100 = 125 (not specified)	EG-Richtlinie 79/831/EWG, C.2 "Acute Toxicity for Daphnia", no further details
Octadecanedioic acid; 871-70-5	*Daphnia magna*	>100 (nominal) exceeds expected water solubility	OECD TG 202, static
	Aquatic plants	**EC_{50} (mg/L), 72 hr**	
Alkyl ranges and source based			
Sponsored substances			
Fatty acids, C14-22; 68424-37-3	*Desmodesmus subspicatus*	>100 (nominal) exceeds expected water solubility	DIN 38412/9
Fatty acids, C14-18 and C16-18-unsaturated; 67701-06-8	*Desmodesmus subspicatus*	51 (nominal; 96 hr) exceeds expected water solubility	DIN 38412/9
Dicarboxylic acids			
Sponsored substances			
Decanedioic acid; 111-20-6	*Desmodesmus subspicatus*	NOEC >=10; EbC50>10; 24 hour ErC50 >10 (nominal)	OECD TG 203
Supporting substances			
Hexanedioic acid; 124-04-9	*Desmodesmus subspicatus*	26.6 (96 hr; nominal/measured not specified)	Algentest in Anlehnung an UBA
Octadecanedioic acid; 871-70-5	*Desmodesmus subspicatus*	EbC50 and ErC50 > 100 (nominal; exceeds expected water solubility); WAF = 0.14-0.19 (measured; limit of expected water solubility)	OECD TG 203

Dodecanedioic acid; 693-23-2	*Desmodesmus subspicatus*	EC_0 >=5.8 (nominal; highest concentration tested) exceeds water solubility	Algentest in Anlehnung an UBA
Sodium and potassium salts			
Sponsored substances			
Fatty acids, C12-18, sodium salts; CAS 91032-12-1	*Desmodesmus subspicatus*	EbC50 = 25; ErC50 = 41 (nominal) exceeds expected water solubility	DIN 38412/9

The Aliphatic Acids category members possess properties indicating a hazard for the environment (acute toxicity to fish: between 1-100 mg/L for carbon chain lengths C6 through C12, and multi-component sodium or potassium salts C16-18; acute toxicity to aquatic invertebrates: between 1 and 100 mg/L for carbon chain lengths C6 through C9 (including sodium salts) and less than 1 mg/L for sodium salts single component aliphatic acids C18 and multi component sodium salt aliphatic acids with carbon chain lengths including C14 through C18; and, acute toxicity to aquatic plants: between 1-100 mg/L for carbon chain length C12, including sodium or ammonium salts). The weight of evidence indicates that the Aliphatic Acids category members are readily biodegradable and are not expected to bioaccumulate. Adequate screening-level data are available to characterize the hazard for the environment for the purposes of the OECD Cooperative Chemicals Assessment Programme.

Exposure

According to the HERA Project Assessment on Fatty Acid Salts (2003), the estimated annual tonnage of fatty acids salts produced for use in household cleaning products in Europe is 71,306 metric tons. This has been compiled from 4 of the 6 main formulator companies and is estimated to cover greater than 80% of the tonnage used in household cleaning products. The total use of fatty acid salts in Europe in 1994 was estimated to be 701,000 MT/year. The estimated regional production volumes of the sponsored category of aliphatic acids, based on a 2002 survey of Consortium member companies (unpublished), are 997,900 tonnes in Europe and 952,500 tonnes in North America.

The textile industry is one of the major industrial and commercial users of fatty acids and their derivatives. Beyond their wetting properties, as are used in neutral soaps, fatty acids are used in dyeing, as textile lubricating agents, and as resins. Fatty acids are also used in pharmaceuticals, lubrication oils, as protective coatings, in rubber manufacturing, mining, metal working and in leather softening.
Aliphatic acids and their salts (soap) are widely used in household cleaning products, cosmetics including many lotions, lipsticks, and cleansing creams, food and food packaging, and paints and coatings.

Environmental exposure could arise in association with production, formulation and industrial use of these substances. There would also be exposure from consumer uses. The majority of the aliphatic acid salt uses result in down the drain releases to the environment.

For routine occupational operations, including those involving a breach of the closed system, goggles or safety glasses, gloves, safety boots and helmets are worn. Aliphatic acids have a low volatility and as a rule engineering controls are available that prevent the need for respiratory protection. Major routes of consumer exposure to aliphatic acids are from the use of aliphatic acid salts (soaps) in bar soaps and in household cleaning products.

Annex 1

Table 1 Summary of Read Across Approach Mammalian Toxicity Data

Substance CAS#	Acute toxicity (oral and inhalation)	Repeated dose (oral)	Gene mutation *in vitro*	Chromosome aberration *in vitro*	Chromosome aberration *in vivo*	Effects on fertility and/or reproductive organs	Developmental toxicity (oral)
Single component – Saturated (12)							
142-62-1	RA to 124-07-2 LD50 oral > 2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	**Negative**	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative))	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
111-14-8	RA to 124-07-2	RA to	**Negative**	WOE Single	WOE	RA to CAS *112-85-*	RA to CAS

	LD50 oral > 2000	*CAS 112-85-6* NOAEL = 1000 (42d)		component saturated (negative)	Dicarboxylic acids (negative))	*6*, NOAEL = 1000 (M/F)	*112-85-6*, NOAEL = 1000 (maternal and developmental)
124-07-2	**LD50 oral > 2000, > 5000, > 14700**	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	**Negative**	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative))	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
112-05-0	RA to CAS 124-07-2 and *112-85-6*; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
334-48-5	**LD50 oral > 10000**	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
143-07-7	**LD50 oral > 5000, > 10000**	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Sponsored and Supporting (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
544-63-8	**LD50 oral > 10000**	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
57-10-3	**LD50 oral > 5000, > 10000**	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
506-12-7	RA to CAS 57-10-3; >5000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Sponsored and Supporting (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
57-11-4	**LD50 oral > 5000, > 10000**	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
30399-84-9	**LD50 oral > 2000**	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	**Negative**	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
106-14-9	RA to CAS 30399-84-9; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	**Negative**	**Negative**	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
Supporting 112-85-6	***LD50 oral > 2000***	***NOAEL = 1000 (42d)***	***Negative***	***Negative***	*No data*	***NOAEL = 1000***	***NOAEL = 1000* (maternal**

							and developmental)
Single component – mono – unsaturated (4)							
544-64-9	RA to CAS 112-80-1; >2000	RA to CAS 112-80-1 NOAEL = 14000 (90d)	RA to 112-80-1 (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M) and *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS 60-33-3 NOEL = 10000
2091-29-4	RA to CAS 112-80-1; >2000	RA to CAS 112-80-1 NOAEL = 14000 (90d)	RA to 112-80-1 (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M) and *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS 60-33-3 NOEL = 10000
112-80-1	**LD50 oral > 2000, > 5000, > 19100**	**NOAEL = 14000 (90d)**	**Negative**	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M) and *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS 60-33-3 NOEL = 10000
112-86-7	**LD50 oral > 5000**	RA to CAS 112-80-1 NOAEL = 14000 (90d)	RA to 112-80-1 (negative)	WOE Single component saturated (negative)	WOE Supporting (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M) and *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS 60-33-3 NOEL = 10000
Single component – di – unsaturated (2)							
60-33-3	RA to CAS 112-80-1; >2000	**NOAEL = 467 – 1970 (M, 36wk)**	**Negative**	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	**NOAEL = 467-1970 (M)**	**NOEL = 10,000**
121250-47-3	RA to CAS 112-80-1; >2000	RA to CAS 60-33-3 NOAEL = 467 – 1970 (M, 36wk), and 112-80-1 NOAEL = 14000 (90d)	RA to 112-80-1 (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M) and *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS 60-33-3 NOEL = 10000
Single component – tri – unsaturated (1)							
463-40-1	RA to CAS 124-07-2 and *112-85-6*; >2000	RA to CAS 60-33-3 NOAEL = 467 – 1970 (M, 36wk), and 112-80-1 NOAEL = 14000 (90d)	RA to 112-80-1 (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M) and *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS 60-33-3 NOEL = 10000
Alkyl range sourced based (multi-component) – Saturated (13)							
68603-84-9	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
68937-74-6	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
67762-36-1	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
68937-75-7	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
90990-08-2	RA to CAS 90990-11-7; >5000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
68002-90-4	RA to CAS 90990-11-7; >5000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and

							developmental)
90990-10-6	RA to CAS 90990-11-7; >5000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
67701-01-3	RA to CAS 90990-11-7; >5000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
67701-02-4	**LD50 oral > 2000**	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
68424-37-3	RA to CAS 90990-11-7; >5000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
67701-03-5	RA to CAS 67701-02-4 and *85711-54-2*; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
68937-76-8	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative))	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
90990-11-7	**LD50 oral > 5000**	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative))	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
Alkyl range sourced based (multi-component) – Unsaturated (1)							
68648-24-8	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
Alkyl range sourced based (multi-component) – Mixture of saturated and unsaturated (16)							
68937-85-9	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative))	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
68938-15-8	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative))	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
61788-47-4	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
67701-05-7	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Sponsored and Supporting (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
68918-39-8	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
90990-15-1	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Sponsored and Supporting (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
68334-03-2	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
61790-38-3	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
67701-06-8	**LD50 oral > 5000**	RA to CAS *61790-12-3*	RA to *61790-12-3* (negative)	WOE Single component	WOE Dicarboxylic	RA to CAS *61790-12-3*,	RA to CAS *61790-12-3*

		NOAEL = 2500 (90d)		saturated (negative)	acids (negative)	NOAEL = 5000 (F0,F1)	NOAEL = 5000
61790-37-2	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
68308-53-2	RA to CAS 67701-02-4 and *85711-54-2*; >2000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
68002-87-9	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
68440-15-3	RA to CAS 67701-02-4 and *85711-54-2*; >2000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
67701-07-9	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
67701-08-0	**LD50 oral > 5000**	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
61789-45-5	RA to CAS 67701-06-8; >5000	RA to CAS *61790-12-3* NOAEL = 2500 (90d)	RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *61790-12-3*, NOAEL = 5000 (F0,F1)	RA to CAS *61790-12-3* NOAEL = 5000
Supporting 61790-12-3	***LD50 oral > 10000***	***NOAEL = 2500 (90d)***	***Negative***	*No data*	*No data*	***NOAEL = 5000 (F0,F1)***	***NOAEL = 5000***
Supporting 85711-54-2	***LD50 oral > 2000***	*No data*	*No data*	*No data*	*No data*	*No data*	*No data*
Dicarboxylic acids (single or multi-component) - Saturated (4)							
Supporting 110-15-6	***LD50 oral = 2260***	***NOAEL = 1700-2100 (13wk)***	***Negative***	***Negative***	*No data*	*No data*	*No data*
Supporting 110-94-1	***LD50 oral = 2750***	***NOAEL = 800 (90d)***	***Negative***	*No data*	***In vivo mouse micronucleus/Negative***	*No data*	***NOAEL (maternal) = 125 Developmental = 1300***
Supporting 124-04-9	***LD50 oral = 5050***	***NOAEL = 2700(M) 63(F) (2yr)***	***Negative***	*No data*	***Negative***	***NOAEL = 2700 (M); 63 (F)***	***NOAEL > 288 (maternal and developmental)***
68937-72-4	RA to CAS 124-04-9; 5050	RA to CAS *110-94-1* NOAEL = 800 (90 d)	WOE Dicarboxylic acids (negative))	WOE Dicarboxylic acids (negative))	WOE Dicarboxylic acids (negative))	RA to CAS *124-04-9* NOAEL = 63 (F) and *693-23-2*, NOAEL = 1000 (M)	RA to CAS *110-94-1* NOAEL = (maternal) = 125 and *124-04-9* (developmental) >288
123-99-9	**LD50 oral > 5000**	RA to CAS *110-94-1* NOAEL = 800 (90 d)	WOE Dicarboxylic acids (negative))	RA to *110-15-6* (negative)	WOE Dicarboxylic acids (negative))	RA to CAS *124-04-9* NOAEL = 63 (F) and *693-23-2*, NOAEL = 1000 (M)	RA to CAS *110-94-1* NOAEL = (maternal) = 125 and *124-04-9* (developmental) >288
111-20-6	**LD50 oral > 2000**	RA to CAS *110-94-1* NOAEL = 800 (90 d)	**Negative**	WOE Dicarboxylic acids (negative))	WOE Dicarboxylic acids (negative))	RA to CAS *124-04-9* NOAEL = 63 (F) and *693-23-2*, NOAEL = 1000 (M)	RA to CAS *110-94-1* NOAEL = (maternal) = 125 and *124-04-9* (developmental) >288
68937-70-2	RA to CAS 111-20-6; >2000	RA to CAS *110-94-1* NOAEL = 800 (90 d)	WOE Dicarboxylic acids (negative))	WOE Dicarboxylic acids (negative))	WOE Dicarboxylic acids (negative))	RA to CAS *124-04-9* NOAEL = 63 (F) and *693-23-2*, NOAEL = 1000 (M)	RA to CAS *110-94-1* NOAEL = (maternal) = 125 and *124-04-9* (developmental) >288

Supporting 693-23-2	***LD50 oral > 3000, > 17000***	***NOAEL = 5000(14d rf), = 1000 (15d)***	***Negative***	*No data*	*No data*	***NOAEL = 1000***	***NOAEL = 1000 (parental and developmental)***
Supporting 871-70-5	***LD50 oral > 5000***	***NOAEL = 1000 (28d), = 1000(14d rf)***	***Negative***	***Negative***	*No data*	*No data*	*No data*
Sodium and potassium salts (single or multi-component) – Saturated (10)							
67762-44-1	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative))	RA to *CAS 112-85-6* NOAEL = 1000	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
1984-06-1	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative))	RA to *CAS 112-85-6* NOAEL = 1000	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
1002-62-6	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative))	RA to *CAS 112-85-6* NOAEL = 1000	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
629-25-4	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative))	RA to *CAS 112-85-6* NOAEL = 1000	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
10124-65-9	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative))	RA to *CAS 112-85-6* NOAEL = 1000	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
91032-12-1	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative))	RA to *CAS 112-85-6* NOAEL = 1000	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
822-12-8	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to *CAS 112-85-6* NOAEL = 1000	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
408-35-5	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to *CAS 112-85-6* NOAEL = 1000	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
68424-38-4	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to *CAS 112-85-6* NOAEL = 1000	RA to CAS Supporting 112-85-6 and 124-04-9
822-16-2	RA to CAS 67701-02-4; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to *CAS 112-85-6* NOAEL = 1000	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
Sodium and potassium salts (single component) Mono-unsaturated (1)							
143-18-0	RA to CAS 112-80-1; >2000	RA to CAS 112-80-1 NOAEL = 14000 (90d)	RA to 112-80-1 (negative)	WOE Sponsored and Supporting (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M) and *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS 60-33-3 NOEL = 10000
Sodium and potassium salts (multi-component) – Mixture of saturated and unsaturated (9)							
61789-30-8	RA to CAS *68424-26-0*; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated and RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M); *112-85-6* and 693-*23-2* , NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
61789-31-9	RA to CAS *68424-26-0*; >2000	RA to *CAS 112-85-6* NOAEL =	WOE Single component saturated and RA to *61790-12-3*	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M); *112-85-6* and	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and

		1000 (42d)	(negative)			693-*23-2* , NOAEL = 1000 (M/F)	developmental)
67701-09-1	RA to CAS *68424-26-0*; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated and RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M); *112-85-6* and 693-*23-2* , NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
67701-10-4	RA to CAS *68424-26-0*; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated and RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M); *112-85-6* and 693-*23-2* , NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
68082-64-4	RA to CAS *68424-26-0*; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated and RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M); *112-85-6* and 693-*23-2* , NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
67701-11-5	RA to CAS *68424-26-0*; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated and RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M); *112-85-6* and 693-*23-2* , NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
8052-48-0	RA to CAS *68424-26-0*; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated and RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M); *112-85-6* and 693-*23-2* , NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
61790-79-2	RA to CAS *68424-26-0*; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated and RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M); *112-85-6* and 693-*23-2* , NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
68002-80-2	RA to CAS *68424-26-0*; >2000	RA to *CAS 112-85-6* NOAEL = 1000 (42d)	WOE Single component saturated and RA to *61790-12-3* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 60-33-3, NOAEL = 467-1970 (M); *112-85-6* and 693-*23-2* , NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
Supporting 68424-26-0	***LD50 oral > 2000***	*No data*	*No data*	*No data*	*No data*	*No data*	*No data*
Magnesium and calcium salts (multi-component) - Mixture Saturated and Unsaturated (1)							
64755-01-7	RA to CAS 557-04-0, >10,000	RA to CAS 557-04-0 NOAEL = 4000 (90 d)	RA to CAS 557-04-0 (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 557-04-0, NOAEL = 4000	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
Magnesium and calcium salts (single component) – Saturated (2)							
542-42-7	RA to CAS 557-04-0, >10,000	RA to CAS 557-04-0 NOAEL = 4000 (90 d)	RA to CAS 557-04-0 (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS 557-04-0, NOAEL = 4000	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
557-04-0	**LD50 oral > 10000 LC50 inh > 2 (60 min)**	**NOAEL = 4000 (90d)**	**Negative**	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	**NOAEL = 4000**	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
Ammonium salts (single component) Saturated (2)							
2437-23-2	RA to CAS *84753-04-8*; >2000	RA to	RA to CAS *84753-04-8* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and

							developmental)
1002-89-7	RA to CAS *84753-04-8*; >2000	*CAS 112-85-6* NOAEL = 1000 (42d)	RA to *84753-04-8* (negative)	WOE Single component saturated (negative)	WOE Dicarboxylic acids (negative)	RA to CAS *112-85-6*, NOAEL = 1000 (M/F)	RA to CAS *112-85-6*, NOAEL = 1000 (maternal and developmental)
Supporting 84753-04-8	***LD50 oral > 2000***	*No data*	***Negative***	*No data*	*No data*	*No data*	*No data*

Multi-component substances presented in red text.

Table 2 Summary of Read Across Approach: Irritation

Substance CAS# (Carbon chain length)	Skin irritation	Eye irritation
Single component – Saturated (12)		
142-62-1 (C6)	**Corrosive**	RA to 124-07-2 Irritating
111-14-8 (C7)	**Irritating**	RA to 124-07-2 Irritating
124-07-2 (C8)	**Corrosive**	**Irritating**
112-05-0 (C9)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
334-48-5 (C10)	**Corrosive**	**Irritating**
143-07-7 (C12)	**Irritating**	**Irritating**
544-63-8 (C14)	**Not irritating**	**Not irritating**
57-10-3 (C16)	**Not irritating**	**Not irritating**
506-12-7 (C17)	RA to 57-10-3 Not irritating	RA to 57-10-3 Not irritating
57-11-4 (C18)	**Not irritating**	**Not irritating**
30399-84-9 (C18, Me branched)	**Irritating**	RA to 57-11-4 Not irritating
106-14-9 (C18 hydroxyl)	RA to 57-11-4 Not irritating	RA to 57-11-4 Not irritating
Supporting 120-87-6 (C18 hydroxyl)	*No data*	***Not irritating***
Single component – mono – unsaturated (4)		
544-64-9 (C14)	RA to 112-80-1 Not irritating	RA to 112-80-1 Not irritating
2091-29-4 (C16)	RA to 112-80-1 Not irritating	RA to 112-80-1 Not irritating
112-80-1 (C18)	**Not irritating**	**Not irritating**
112-86-7 (C22)	**Mildly irritating**	**Not irritating**
Single component – di – unsaturated (2)		
60-33-3 (C18)	RA to 112-80-1 Not irritating	RA to 112-80-1 Not irritating
121250-47-3 (C18)	RA to 112-80-1 Not irritating	RA to 112-80-1 Not irritating
Single component – tri – unsaturated (1)		
463-40-1 (C18)	RA to 112-80-1 Not irritating	RA to 112-80-1 Not irritating
Alkyl range sourced based (multi-component) – Saturated (13)		
68603-84-9 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
68937-74-6 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
67762-36-1 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
68937-75-7 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
90990-08-2 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
68002-90-4 (NA)	RA to 334-48-5 Corrosive	RA to 334-48-5 Irritating
90990-10-6 (NA)	RA to 143-07-7 Irritating	RA to 143-07-7 Irritating

67701-01-3 (NA)	RA to 143-07-7 Irritating	RA to 143-07-7 Irritating
67701-02-4 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
68424-37-3 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
67701-03-5 (NA)	RA to 57-10-3 Not irritating	RA to 57-10-3 Not irritating
68937-76-8 **(NA)**	RA to 57-10-3 Not irritating	RA to 57-10-3 Not irritating
90990-11-7 **(NA)**	RA to 57-11-4 Not irritating	RA to 57-11-4 Not irritating
Alkyl range sourced based (multi-component) – Unsaturated (1)		
68648-24-8 (NA)	RA to 143-07-7 Irritating	RA to 143-07-7 Irritating
Alkyl range sourced based (multi-component) – Mixture of saturated and unsaturated (16)		
68937-85-9 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
68938-15-8 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
61788-47-4 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
67701-05-7 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
68918-39-8 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
90990-15-1 (NA)	RA to 143-07-7 Irritating	RA to 143-07-7 Irritating
68334-03-2 (NA)	RA to 143-07-7 Irritating	RA to 143-07-7 Irritating
61790-38-3 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
67701-06-8 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
61790-37-2 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
68308-53-2 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
68002-87-9 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
68440-15-3 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
67701-07-9 (NA)	RA to 57-10-3 Not irritating	RA to 57-10-3 Not irritating
67701-08-0 (NA)	**Not irritating**	**Not irritating**
61789-45-5 (NA)	RA to 57-11-4 Not irritating	RA to 57-11-4 Not irritating
Dicarboxylic acids (single or multi-component) – Saturated (4)		
Supporting 110-15-6 (C4)	RA to 110-94-1 Not irritating	**Severe irritant**
Supporting 110-94-1 (C5)	**Not irritating**	**Irritating**
Supporting 124-04-9 (C6)	**Not irritating**	**Irritating**
68937-72-4 (NA)	RA to 110-94-1 Not irritating	RA to 110-15-6 Severe irritant
123-99-9 (C9)	**Not irritating**	RA to 124-04-9 Irritating
111-20-6 (C10)	RA to 123-99-9 Not irritating	RA to 124-04-9 Irritating
68937-70-2 (NA)	RA to 124-04-9 Not irritating	RA to 124-04-9 Irritating
Supporting 871-70-5 (C18)	*No data*	***Irritating***
Sodium and potassium salts (single or multi-component) – Saturated (10)		
67762-44-1 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
1984-06-1 (C8)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
1002-62-6 (C10)	RA to 334-48-5 Corrosive	RA to 334-48-5 Irritating
629-25-4 (C12)	RA to 143-07-7 Irritating	RA to 143-07-7 Irritating

10124-65-9 (C12)	RA to 143-07-7 Irritating	RA to 143-07-7 Irritating
91032-12-1 (NA)	RA to 143-07-7 Irritating	RA to 143-07-7 Irritating
822-12-8 (C14)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
408-35-5 (C16)	RA to 57-10-3 Not irritating	RA to 57-10-3 Not irritating
68424-38-4 (NA)	RA to 57-10-3 Not irritating	RA to 57-10-3 Not irritating
822-16-2 (C18)	RA to 57-11-4 Not irritating	RA to 57-11-4 Not irritating
Sodium and potassium salts (single component) Mono-unsaturated (1)		
143-18-0 (C18)	RA to 57-11-4 Not irritating	RA to 57-11-4 Not irritating
Sodium and potassium salts (multi-component) – Mixture of saturated and unsaturated (9)		
61789-30-8 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
61789-31-9 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
67701-09-1 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
67701-10-4 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
68082-64-4 (NA)	RA to 124-07-2 Corrosive	RA to 124-07-2 Irritating
67701-11-5 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
8052-48-0 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
61790-79-2 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
68002-80-2 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
Magnesium and calcium salts (multi-component) - Mixture Saturated and Unsaturated (1)		
64755-01-7 (NA)	RA to 544-63-8 Not irritating	RA to 544-63-8 Not irritating
Magnesium and calcium salts (single component) – Saturated (2)		
542-42-7 (C16)	RA to 557-04-0 Not irritating	RA to 557-04-0 Not irritating
557-04-0 (C18)	**Not irritating**	**Not irritating**
Ammonium salts (single component) Saturated (2)		
2437-23-2 (C12)	RA to 143-07-7 Irritating	RA to 84753-04-8 Corrosive
1002-89-7 (C18)	RA to 84753-04-8 Not irritating	RA to 84753-04-8 Corrosive
Supporting 84753-04-8 (C18)	***Not irritating***	***Corrosive***

Multi-component substances presented in red text.

Table 3 Summary of Read Across Approach: Biodegradation and Aquatic Toxicity

Substance CAS#	**Water Solubility (mg/L at 25 °C)**	**Biodegradation**	**Fish mg/L (96 h LC50)** [ECOSAR]	**Daphnia mg/L (48 h EC50)** [ECOSAR]	**Algae mg/L (72 h EC50)** [ECOSAR]
Single component – Saturated (12)					
142-62-1	1.03+04 (measured)	RA to 124-07-2 (Readily biodegradable)	**320 (measured) (>100)**	RA to 124-04-9 85.7 (nominal)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects (no hazard at the solubility limit of the test)
111-14-8	2820 (modeled)	RA to 124-07-2 (Readily biodegradable)	RA to 124-07-2 48 h: 57 (nominal)	RA to 124-04-9 85.7 (nominal)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects

					(no hazard at the solubility limit of the test)
124-07-2	789 at 30°C (measured)	**Readily biodegradable**	**48 h: 57 (nominal)**	RA to 124-04-9 85.7 (nominal)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects (no hazard at the solubility limit of the test)
112-05-0	284 at 20°C (measured)	**Readily biodegradable**	**104 (measured)**	RA to 124-04-9 85.7 (nominal)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects (no hazard at the solubility limit of the test)
334-48-5	61.8 (measured)	RA to 112-05-0 (Readily biodegradable)	**48 h: 20 (nominal)**	RA to 111-20-6 >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects) (no hazard at the solubility limit of test)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects (no hazard at the solubility limit of the test)
143-07-7	4.81 (measured)	**Biodegradable**	**150* (nominal)**	**5.6 mg/L (measured) (WAF, single conc tested; prepared at a Loading Level of 10,000 mg/L**	RA to 693-23-2 EC0 > 5.8 (limit test: highest conc tested was at the WS limit for the test)
544-63-8	1.07 (measured)	RA to 143-07-7 (Biodegradable)	**>100 - < 300* (nominal)**	RA to 61790-38-3 EC0>100* (nominal)	RA to 68242-37-3 >100* (nominal)
57-10-3	0.04 (measured)	**Ultimately biodegradable**	**>1000* (nominal)**	RA to 61790-38-3 EC0>100* (nominal)	RA to 68242-37-3 >100* (nominal)
506-12-7	0.0195 (modeled)	RA to 57-11-4 (Biodegradable)	RA to 57-10-3 >1000* (nominal)	RA to 61790-38-3 EC0>100* (nominal)	RA to 68242-37-3 >100* (nominal)
57-11-4	0.597 (measured)	**Biodegradable**	**>1000* (nominal)**	RA to 112-80-1 EC_0>32* (nominal; no effect at highest conc tested	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
30399-84-9	0.007 (modeled)	**Biodegradable**	**48 h: 13.4* (nominal)**	RA to 112-80-1 EC_0>32* (nominal; no effect at highest conc tested	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
106-14-9	0.3315 (modeled)	**Readily biodegradable**	RA to 120-87-6 *>10000 (nominal)**	RA to 112-80-1 EC_0>32* (nominal; no effect at highest conc tested	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
Supporting 120-87-6	*0.7641 (modeled)*	*No data*	***>10000 (nominal)****	*No data*	*No data*
Single component – mono – unsaturated (4)					
544-64-9	0.94 (modeled)	WOE Single component – mono - unsaturated (readily biodegradable)	RA to 544-63-8 >100 - < 300* (nominal)	RA to 61790-38-3 EC0>100* (nominal)	RA to 68242-37-3 >100* (nominal)

2091-29-4	0.13 (modeled)	WOE Single component – mono - unsaturated (readily biodegradable)	RA to C16 (57-10-3) >1000* (nominal)	RA to 61790-38-3 EC0>100* (nominal)	RA to 68242-37-3 >100* (nominal)
112-80-1	0.01151 (modeled)	**Readily biodegradable**	**>56* (nominal)**	**EC_0>32* (nominal; no effect at highest conc tested**	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
112-86-7	9.491E-05 (modeled)	**Readily biodegradable**	RA to C18 (112-80-1) >56* (nominal)	RA to 112-80-1 EC_0>32* (nominal; no effect at highest conc tested	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
Single component – Di-unsaturated (2)					
60-33-3	C18, 2 double bond; 0.03771 (modeled)	**Biodegradable**	RA to C18 (112-80-1) >56* (nominal)	**55* (nominal, WAF that exceeded WS limit)**	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
121250-47-3	0.0377 (modeled)	RA to 60-33-3 (biodegradable)	RA to C18 (112-80-1) >56* (nominal)	RA to 60-33-3 55* (nominal, WAF that exceeded WS limit)	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
Single component – Tri-unsaturated (1)					
463-40-1	0.124 (modeled)	RA to 60-33-3 (biodegradable)	RA to C18 (112-80-1) >56* (nominal)	RA to 60-33-3 55* (nominal, WAF that exceeded WS limit)	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
Alkyl range sourced based (multi-component) – Saturated (13)					
68603-84-9	1.03E+04 (measured)	RA to 68424-37-3 (moderately biodegradable)	RA to 124-07-2 48 h: 57 (nominal)	RA to 124-04-9 85.7 (nominal)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
68937-74-6	C6: 1.03E+04 (measured) – C10: 61.8 (measured)	RA to 68424-37-3 (moderately biodegradable)	RA to 334-48-5 48 h: 20 (nominal)	RA to 124-04-9 85.7 (nominal)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
67762-36-1	C6: 1.03E+04 (measured) - C12: 4.81 (measured)	RA to 68424-37-3 (moderately biodegradable)	**38 (nominal)**	RA to 124-04-9 85.7 (nominal)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
68937-75-7	C8: 789 at 30 °C – C10: 61.8 (measured)	RA to 68424-37-3 (moderately biodegradable)	RA to 334-48-5 48 h: 20 (nominal)	RA to 111-20-6 >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
90990-08-2	C8: 789 at 30 °C – C18: 0.597 (measured)	RA to 68424-37-3 (moderately biodegradable)	RA to 334-48-5 48 h: 20 (nominal)	RA to 111-20-6 >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
68002-90-4	C10: 6.18 (measured) – C16: 0.04 (measured)	RA to 68424-37-3 (moderately biodegradable)	RA to 334-48-5 48 h: 20 (nominal)	RA to 111-20-6 >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
90990-10-6	C12: 4.81 (measured) – C14: 1.07 (measured)	RA to 68424-37-3 (moderately biodegradable)	RA to 143-07-7 150* (nominal)	RA to 143-07-7 5.6 mg/L (measured) (WAF, single conc tested; prepared at a Loading Level of 10,000	RA to 693-23-2 EC0 > 5.8 (limit test: highest conc tested was at the WS limit for the

				mg/L	test)
67701-01-3	C12: 4.81 – C18: 0.597 (measured)	RA to 68424-37-3 (moderately biodegradable)	RA to 143-07-7 150* (nominal) (>100)	RA to 143-07-7 5.6 mg/L (measured) (WAF, single conc tested; prepared at a Loading Level of 10,000 mg/L	RA to 693-23-2 EC0 > 5.8 (limit test: highest conc tested was at the WS limit for the test)
67701-02-4	C14: 1.07 – C18: 0.597 (measured)	RA to 68424-37-3 (moderately biodegradable)	RA to 544-63-8 >100 - < 300* (nominal)	RA to 61790-38-3 EC0>100* (nominal)	RA to 67701-06-8 96 h: 51* (nominal)
68424-37-3	C14: 1.07 (measured) – C22: 0.016 (modeled)	**Moderately biodegradable**	RA to 544-63-8 >100 - < 300* (nominal)	RA to 61790-38-3 EC0>100* (nominal)	**>100* (nominal)**
67701-03-5	C16: 0.04 (measured) – C18: 0.597 (measured)	RA to 68424-37-3 (moderately biodegradable)	**48 h: >1000* (nominal)**	RA to 95912-82-6 >0.695 (measured WAF; corresponds to 1020 mg/L nominal)	RA to 67701-06-8 96 h: 51* (nominal)
68937-76-8	C16: 0.04 (measured) – C20 3E-04 (modeled)	RA to 68424-37-3 (moderately biodegradable)	RA to 67701-03-5 48 h: >1000* (nominal)	RA to 95912-82-6 >0.695 (measured WAF; corresponds to 1020 mg/L nominal)	RA to 67701-06-8 96 h: 51* (nominal)
90990-11-7	C18: 0.597 (measured) – C22 0.016 (modeled)	RA to 68424-37-3 (moderately biodegradable)	**>100* (nominal)**	RA to 60-33-3 55* (nominal, WAF that exceeded WS limit)	RA to 68424-37-3 >100* (nominal)
Alkyl range sourced based (multi-component) – Unsaturated (1)					
68648-24-8	C12:1 9.12 – C20:1 9.61 E-04 (modeled)	RA 68424-37-3 (moderately biodegradable)	RA to 143-07-7 150* (nominal)	RA to 143-07-7 5.6 mg/L (measured) (WAF, single conc tested; prepared at a Loading Level of 10,000 mg/L	RA to 693-23-2 EC0 > 5.8 (limit test: highest conc tested was at the WS limit for the test)
Alkyl range sourced based (multi-component) – Mixture of saturated and unsaturated (16)					
68937-85-9	C8: 789 at 30 °C – C12: 4.81 (measured)	RA to 143-07-7 (biodegradable)	RA to 334-48-5 48 h: 20 (nominal)	RA to 111-20-6 >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
68938-15-8	C8: 789 at 30 °C – C12: 4.81 (measured)	RA to 143-07-7 (biodegradable)	RA to 334-48-5 48 h: 20 (nominal)	RA to 111-20-6 >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
61788-47-4	C8: 789 at 30 °C – C12: 4.81 (measured)	RA to 143-07-7 (biodegradable)	RA to 334-48-5 48 h: 20 (nominal)	RA to 111-20-6 >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
67701-05-7	C8: 789 at 30 °C – C18: 0.597 (measured) C18:1 0.0115 C18:2a 0.0377 C18:2b 0.0377 C18:3 0.124 (modeled)	RA to 57-11-4 (biodegradable)	RA to 334-48-5 48 h: 20 (nominal)	RA to 111-20-6 >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
68918-39-8	C8: 789 at 30 °C – C18: 0.597 (measured) C18:1 0.0115 C18:2a 0.0377 C18:2b 0.0377 C18:3 0.124 (modeled)	RA to 57-11-4 (biodegradable)	RA to 334-48-5 48 h: 20 (nominal)	RA to 111-20-6 >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
90990-15-1	C12: 4.81 –C18: 0.597 (measured) C18:1 0.0115 C18:2 8.17	RA to 143-07-7 (biodegradable)	RA to 143-07-7 150* (nominal)	RA to 143-07-7 5.6 mg/L (measured) (WAF, single conc tested; prepared at a	RA to 693-23-2 EC0 > 5.8 (limit test: highest conc tested was at the

	C18:2a 0.0377 C18:2b 0.0377 C18:3 0.124 (modeled)			Loading Level of 10,000 mg/L	WS limit for the test)
68334-03-2	C12: 4.81 (measured) – C20: 3E-04 (modeled) C12:1 9.12 - C20:1 9.611E-04 (modeled)	RA to 143-07-7 (biodegradable)	RA to 143-07-7 150* (nominal)	RA to 143-07-7 5.6 mg/L (measured) (WAF, single conc tested; prepared at a Loading Level of 10,000 mg/L	RA to 693-23-2 EC0 > 5.8 (limit test: highest conc tested was at the WS limit for the test)
61790-38-3	C14: 1.07 – C18 0.597 (measured)	RA to 61790-37-2 (biodegradable)	RA to 61790-37-2 >100* (nominal)	**EC0>100* (nominal)**	RA to 67701-06-8 96 h: 51* (nominal)
67701-06-8	C14: 1.07 – C18: 0.597 (measured) C18:1 0.0115 C18:2a 0.0377 C18:2b 0.0377 C18:3 0.124 (modeled)	**Readily biodegradable**	**>1000* (nominal)**	RA to 61790-38-3 EC0>100* (nominal)	**96 h: 51* (nominal)**
61790-37-2	C14: 1.07 – C18: 0.597 (measured) C16:1 0.133 C18:1 0.0115 C18:2a 0.0377 C18:2b 0.0377 C18:3 0.124 (modeled)	**Biodegradable**	**>100* (nominal)**	RA to 61790-38-3 EC0>100* (nominal)	RA to 67701-06-8 96 h: 51* (nominal)
68308-53-2	C14: 1.07 – C18: 0.597 (measured) C18:1 0.0115 C18:2a 0.0377 C18:2b 0.0377 C18:3 0.124 (modeled)	RA to 61790-37-2 (biodegradable)	RA to 61790-37-2 >100* (nominal)	RA to 61790-38-3 EC0>100* (nominal)	RA to 67701-06-8 96 h: 51* (nominal)
68002-87-9	C14: 1.07 (measured) – C22: 9.491E-05 (modeled)	RA to 61790-37-2 (biodegradable)	RA to 61790-37-2 >100* (nominal)	RA to 61790-38-3 EC0>100* (nominal)	RA to 68242-37-3 >100* (nominal)
68440-15-3	C14: 1.07 – C18: 0.597 (measured) C18:1 0.0115 C18:2a 0.0377 C18:2b 0.0377 (modeled)	RA to 61790-37-2 (biodegradable)	RA to 61790-37-2 >100* (nominal)	RA to 61790-38-3 EC0>100* (nominal)	RA to 67701-06-8 96 h: 51* (nominal)
67701-07-9	C16: 0.04 (measured) – C18:1 0.0115 C18:2a 0.0377 C18:2b 0.0377 C18:3 0.124 (modeled)	RA to 61790-37-2 (biodegradable)	RA to 67701-08-0 300* (nominal)	RA to 95912-82-6 >0.695 (measured WAF; corresponds to 1020 mg/L nominal)	RA to 67701-06-8 96 h: 51* (nominal)
67701-08-0	C16: 0.04 (measured) – C18: 0.597 (measured) C18:1 0.0115 C18:2a 0.0377 C18:2b 0.0377 C18:3 0.124 (modeled)	RA to 61790-37-2 (biodegradable)	**300* (nominal)**	RA to 95912-82-6 >0.695 (measured WAF; corresponds to 1020 mg/L nominal)	RA to 67701-06-8 96 h: 51* (nominal)
61789-45-5	C18: 1 0.0115 C18:2a 0.0377 C18:2b 0.0377 (modeled)	RA to 57-11-4 (biodegradable)	RA to C18 (112-80-1) >56* (nominal)	RA to 112-80-1 EC_0>32* (nominal; no effect at highest conc tested	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
Supporting 95912-82-6	*Poorly soluble*	*No data*	*No data*	***>0.695 (measured WAF; corresponds to 1020 mg/L nominal)***	*No data*
Supporting 61790-12-3	*0.01151 (estimated)*	*No data*	*No data*	*No data*	*No data*
Supporting 85711-54-2	*9.491E-5 (estimated)*	*No data*	*No data*	*No data*	*No data*
Supporting 68953-27-5	*.01513 (estimated)*	*No data*	***110 (nominal)***	*No data*	*No data*
Dicarboxylic acids (single or multi-component) – Saturated (4)					
Supporting 110-15-6	*8.079E5 (measured, Epi EDB)*	*No data*	*No data*	**374.2 (nominal)**	*No data*
Supporting 124-04-9	*3.08E4 (measured, Epi EDB)*	*No data*	***97 (nominal)***	***85.7 (nominal)***	*No data*
68937-72-4	1.19E + 04 (measured)	**Readily biodegradable**	*RA to 124-04-9 97 (nominal)*	RA to 110-15-6 374.2 (nominal)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects

123-99-9	2400 at 20 °C (measured)	**Readily biodegradable**	*RA to 124-04-9 97 (nominal)*	RA to 124-04-9 85.7 (nominal)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
111-20-6	1000 at 20 °C (measured)	**Readily biodegradable**	**>9.7 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)**	**>11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)**	**24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects**
68937-70-2	1.03 E+04 (measured)	**Readily biodegradable**	*RA to 124-04-9 97 (nominal)*	RA to 124-04-9 85.7 (nominal)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
Supporting 693-23-2	*40 (measured)*	*No data*	*No data*	*No data*	***$EC_0 \geq$ 5.8 (limit test: highest conc tested was at the WS limit for the test)***
Supporting 871-70-5	*0.1485 (modeled)*	*No data*	***> 100* (nominal, WAF loading level of 100; WAF 0.14-0.22, measured)***	***>100* (nominal)***	***>100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)***
Sodium and potassium salts (single or multi-component) – Saturated (10)					
67762-44-1	C6 1E+06 - C12 3244 (modeled)	RA to 68424-37-3 (moderately biodegradable)	RA to 1984-06-1 310 (nominal)	RA to 124-04-9 85.7 (nominal)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
1984-06-1	9.7 E+05 (modeled)	RA 124-07-2 (readily biodegradable)	**310 (nominal)**	RA to 124-04-9 85.7 (nominal)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
1002-62-6	3.13 E+04 (modeled)	RA 112-05-0 (readily biodegradable)	**54 (nominal; WAF used to test conc <u>above</u> WS limit)**	*RA to 111-20-6* >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 111-20-6 24 h: >10 (nominal), maximum conc tested at limit of solubility; no effects
629-25-4	3244 (modeled)	RA to 143-07-7 (biodegradable)	**11 (nominal; WAF used to test conc <u>above</u> WS limit)**	*RA to 111-20-6* >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 91032-12-1 EbC50 = 25; ErC50 = 41 (nominal)
10124-65-9	2656 (modeled)	RA to 143-07-7 (biodegradable)	RA to 629-25-4 11 (nominal; WAF used to test conc above WS limit)	*RA to 111-20-6* >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 91032-12-1 EbC50 = 25; ErC50 = 41 (nominal)
91032-12-1	C12 3244-C18 3.32	RA *to 91032-09* (readily biodegradable)	RA to 629-25-4 11 (nominal; WAF used to test conc above WS limit)	*RA to 111-20-6* >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	**EbC50 = 25; ErC50 = 41 (nominal)**
Supporting 91032-02-9	**C12-18, potassium**	**Readily biodegradable**	*No data*	*No data*	*No data*
822-12-8	330.8 (modeled)	RA to 143-07-7 (biodegradable)	**118 (nominal)**	*RA to 111-20-6* >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 693-23-2 EC0 > 5.8 (limit test: highest conc tested was at the WS limit for the test)

408-35-5	33.3 (modeled)	**Anaerobically biodegradable**	**150* (nominal)**	*RA to 111-20-6* >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 693-23-2 EC0 > 5.8 (limit test: highest conc tested was at the WS limit for the test)
68424-38-4	C16 33.3 - C18 3.32 (modeled)	RA to 408-35-5 (Anaerobically biodegradable)	RA to 822-16-2 125* (nominal)	RA to 822-16-2 0.57 (nominal)	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
822-16-2	3.32 (modeled)	RA to 57-11-4 (biodegradable)	**125* (nominal)**	RA to 143-18-0 0.57 (nominal)	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
Sodium and potassium salts (single component) - mono-Unsaturated (1)					
143-18-0	4.19 (modeled)	RA to 112-80-1 (readily biodegradable)	**23 (not specified)**	**0.57 (nominal)**	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
Sodium and potassium salts (multi-component) – Mixture of saturated and unsaturated (9)					
61789-30-8	C8 2.48E+05 - C12 2656 (modeled)	RA to 143-07-7 (biodegradable)	RA to 629-25-4 11 (nominal; WAF used to test conc above WS limit)	RA to 124-04-9 85.7 (nominal)	RA to 91032-12-1 EbC50 = 25; ErC50 = 41 (nominal)
61789-31-9	C8 9.67E+05 - C12 3244 (modeled)	RA to 143-07-7 (biodegradable)	RA to 629-25-4 11 (nominal; WAF used to test conc above WS limit)	RA to 124-04-9 85.7 (nominal)	RA to 91032-12-1 EbC50 = 25; ErC50 = 41 (nominal)
67701-09-1	C8 2.48E+05 - C18 2.67 C18:1 4.19 (modeled)	RA to 57-11-4 (biodegradable)	RA to 629-25-4 11 (nominal; WAF used to test conc above WS limit)	RA to 124-04-9 85.7 (nominal)	RA to 91032-12-1 EbC50 = 25; ErC50 = 41 (nominal)
67701-10-4	C8 9.67E+05- C18 3.32 C18:1 5.21 (modeled) C18:2 8.17	RA to 57-11-4 (biodegradable)	RA to 629-25-4 11 (nominal; WAF used to test conc above WS limit)	RA to 124-04-9 85.7 (nominal)	RA to 91032-12-1 EbC50 = 25; ErC50 = 41 (nominal)
68082-64-4	C8 9.67E+05 - C18 3.32 C18:1 5.21 (modeled) C18:2 8.17	RA to 57-11-4 (biodegradable)	RA to 629-25-4 11 (nominal; WAF used to test conc above WS limit)	RA to 124-04-9 85.7 (nominal)	RA to 91032-12-1 EbC50 = 25; ErC50 = 41 (nominal)
67701-11-5	C14 331- C18 3.32 C18:1 5.21 (modeled) C18:2 8.17	RA to 61790-37-2 (biodegradable)	RA to 822-12-8 118 (nominal)	RA to 143-18-0 0.57 (nominal)	RA to 67701-06-8 96 h: 51* (nominal)
8052-48-0	C14 331- C18 3.32 C18:1 5.21 C18:2 8.17 (modeled)	RA to 61790-37-2 (biodegradable)	RA to 822-12-8 118 (nominal)	RA to 143-18-0 0.57 (nominal)	RA to 67701-06-8 96 h: 51* (nominal)
61790-79-2	C14 331- C18 3.32 C18:1 5.21 C18:2 8.17 (modeled)	RA to 61790-37-2 (biodegradable)	RA to 822-12-8 118 (nominal)	RA to 143-18-0 0.57 (nominal)	RA to 67701-06-8 96 h: 51* (nominal)
68002-80-2	C16 26.9- C18 2.67 C18:1 4.19 (modeled)	RA to 68424-37-3 (moderately biodegradable)	*RA to 68424-26-0 54 (nominal)*	RA to 143-18-0 0.57 (nominal)	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
Supporting 68424-26-0	*Likely very soluble*	*No data*	***54 (nominal)***	*No data*	*No data*
Magnesium and calcium salts (Multi-component, Mixture saturated and unsaturated) (1)					

64755-01-7	C14: 9.97E-07 (modeled) - C18: 2.00 at 35°C (measured) C18:1 2.04E-10 (modeled)	RA to 61790-37-2 (biodegradable)	RA to 544-63-8 >100 - < 300* (nominal)	RA to 61790-38-3 EC0>100* (nominal)	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
Magnesium and calcium salts (single component) – Saturated (2)					
542-42-7	9.1 E-09 (modeled)	RA to 57-10-3 (Ultimately biodegradable)	RA to 57-10-3 >1000* (nominal)	RA to 61790-38-3 EC0>100* (nominal)	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
557-04-0	1.045 E-10 (modeled)	RA to 57-11-4 (Biodegradable)	RA TO 30399-84-9 48 h: 13.4* (nominal)	RA to 112-80-1 EC_0>32* (nominal; no effect at highest conc tested	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)
Ammonium salts (single component) – Saturated (2)					
2437-23-2	163.1 (modeled)	143-07-7 (Biodegradable)	RA to 629-25-4 11 (nominal; WAF used to test conc above WS limit)	RA to 143-07-7 >11.6 (measured) (15 nominal, maximum conc tested at limit of solubility; no effects)	RA to 91032-12-1 EbC50 = 25; ErC50 = 41 (nominal)
1002-89-7	0.565 (modeled)	RA to 57-11-4 (Biodegradable)	RA to 822-16-6 125* (nominal)	RA to 112-80-1 EC_0>32* (nominal; no effect at highest conc tested	RA to 871-70-5 >100* (nominal WAF loading level of 100; WAF = 0.14-0.19 measured)

Multi-component substances presented in red text.