SUCROSE MONOESTERS OF LAURIC, PALMITIC OR STEARIC ACID

Chemical and Technical Assessment

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1. Summary

Sucrose monoesters of lauric, palmitic or stearic acid consist mainly of sucrose monoesters of individual fatty acids, namely lauric, palmitic or stearic acid with smaller amounts of the di-esters. They are manufactured by a transesterification reaction of sucrose and vinyl esters of the subject fatty acids. The reaction conditions limit the products primarily to the monoester compounds. Potential trace impurities are removed by a series of distillation and solvent extraction steps. These products have a high emulsifying capacity and thus are used in beverage applications as emulsifiers at low concentrations.

The Committee established a group ADI of 0-30 mg/kg bw for Sucrose monoesters of lauric, palmitic or stearic acid together with sucrose esters of fatty acids, sucroglycerides, sucrose oligoesters type I and sucrose oligoesters type II and the new tentative specifications were prepared at the 73rd JECFA (2010). The specifications were revised and the tentative status was removed at the 74th JECFA (2011).

2. Description

Sucrose monoesters of lauric, palmitic or stearic acid consist mainly monoesters of lauric, palmitic or stearic acid with smaller amounts of its diesters. They appear white to off white powder. They have a high hydrophobic hydrophilic balance (HLB) value that gives them a high emulsifier efficacy. The sucrose monoesters of lauric acid, palmitic acid or stearic acid have excellent emulsifying properties and are used at low levels to emulsify flavours, colours and nutraceutical ingredients (e.g., omega-3 oils) to produce a number of clear beverage products.

They are manufactured by a transesterification reaction between sucrose and vinyl esters of the following specific fatty acids: lauric acid, palmitic acid or stearic acid. This manufacturing process is different from the processes for sucrose esters of fatty acids. As a consequence of the manufacturing process, several trace impurities may be found in the final purified products. These include vinyl laurate, vinyl palmitate or vinyl stearate as starting materials, acetaldehyde formed by tautomerization of vinyl alcohol released in the transesterification reaction and residues of solvents used in the manufacturing process.

3. Manufacturing

The basic raw materials for the manufacture of sucrose monoesters of lauric, palmitic and stearic acid preparations are high purity sucrose (>99.9%) and high purity vinyl fatty acid esters of lauric acid (99%), stearic acid (95%) or palmitic acid (95%).

The manufacturing process involves the initial reaction of sucrose with the fatty acid esters (via transesterification) using a basic catalyst. The reaction step is followed by a series of purification steps to remove the fatty acid vinyl ester starting materials, reaction solvents and other impurities. The purification steps utilize conventional chemical processing methods, such as distillation, solvent extraction and filtration. The only solvents used in the manufacture are dimethyl sulfoxide (DMSO) and isobutanol. The final product is dried into a powder and packaged in hermetically sealed containers.

4. Chemical Characterization

Tables 1-3 show analytical data mainly according to the specifications for “sucrose esters of fatty acids” in several different manufacturing lots of final products, sucrose monoesters of lauric, palmitic or stearic acid.

Table 1. Result of Chemical Analysis for Sucrose Monolaurate Manufacturing Lots

Specification Parameter	Specification	Manufacturing Lots		
		MT09L001	**MT10A001**	**MTA10002**
Assay (%)	> 80	94.5	94.9	93.1
Monoester content (% ot total esters)	-	92.1	94.3	94.0
Diester content (% ot total esters)	-	7.9	5.7	6.0
Fatty acid	Positive	Positive	Positive	Positive
Sugars	Positive	Positive	Positive	Positive
Acid value	< 6	0.35	0.72	0.85
Free sucrose (%)	< 5	1.92	0.93	1.65
Sulfated ash (%)	< 2	0.7	0.4	0.7
Arsenic (mg/kg)	<2	<2	<2	<2
Lead (mg/kg)	<2	<2	<2	<2
Dimethylsulfoxide (mg/kg)	< 2	<2	<2	<2
Isobutanol (mg/kg)	<10	<10	<10	<10

Table 2. Results of Chemical Analysis for Sucrose Monopalmitate Manufacturing Lots

Specification Parameter	Specification	Manufacturing Lots				
		SII09F013	**SII09F014**	**SII09G002**	**SII09G003**	**SII09G004**
Assay (%)	> 80	95.4	94.6	94.3	93.2	92.8
Monoester content (% of total esters)	-	91.1	91.1	91.4	90.9	90.4
Diester content (% of total esters)	-	8.9	8.9	8.6	9.1	9.6
Fatty acid	Positive	Positive	Positive	Positive	Positive	Positive
Sugars	Positive	Positive	Positive	Positive	Positive	Positive
Acid value	< 6	0.23	0.17	0.29	0.29	0.35
Free sucrose (%)	< 5	1.14	1.19	0.90	1.97	1.11
Sulfated ash (%)	< 2	0.6	0.6	0.6	0.6	0.7
Arsenic (mg/kg)	<0.3	<2	<2	<2	<2	<2
Lead (mg/kg)	<2	<2	<2	<2	<2	<2
Dimethylsulfoxide (mg/kg)	< 2	<2	<2	<2	<2	<2
Isobutanol (mg/kg)	<10	<10	<10	<10	<10	<10

Table 3. Results of Chemical Analysis for Sucrose Monostearate Manufacturing Lots

Specification Parameter	Specification	Manufacturing Lots		
		MT10A003	**MT10A004**	**MT10A005**
Assay (%)	> 80	90.1	92.4	90.0
Monoester content (% of total esters))	-	93.0	93.0	92.6
Dister content (% of total esters))	-	7.0	7.0	7.4
Fatty acid	Positive	Positive	Positive	Positive
Sugars	Positive	Positive	Positive	Positive
Acid value	< 6	0.88	0.56	1.12
Free sucrose (%)	< 5	1.17	1.82	1.80
Sulfated ash (%)	< 2	0.8	0.5	0.7
Arsenic (mg/kg)	<2	<2	<2	<2
Lead (mg/kg)	<2	<2	<2	<2
Dimethylsulfoxide (mg/kg)	< 2	<2	<2	<2
Isobutanol (mg/kg)	<10	<10	<10	<10

4.1 Composition

Sucrose monoesters of lauric, palmitic or stearic acid are composed mainly of sucrose monoesters of individual fatty acids, namely lauric acid, palmitic acid or stearic acid with smaller amounts of the diesters. The ratio of diesters depends on the reaction conditions of the transesterification reaction. Although the content of total sucrose esters are generally greater than 90%, the level of monoester varies slightly among the different individual fatty acid products (lauric, palmitic or stearic acid products). Monoesters range from approximately 83% (stearic) to 90% (lauric) and thus, the amounts of diesters range from approximately 6.2% (lauric) to 8.5% (palmitic). Thus the total amount of sucrose fatty acid ester in each product is significantly higher than 80% purity level, which is the minimum level required in the existing specifications for "sucrose esters of fatty acids".

4.2 Possible impurities

Final products of sucrose monoesters of lauric, palmitic or stearic acid contain similar impurities to those in the existing sucrose esters of fatty acids. Free sucrose which is a starting material is from 0.90% to 1.92% and these are adequately lower than the required limits in the existing specifications for "sucrose esters of fatty acids". The residual levels of the solvents, dimethylsulfoxide and isobutanol, used in the manufacturing process are less than 2 and 10 mg/kg, respectively. The levels of arsenic and lead are both less than 2 mg/kg.

The following three additional impurities can be present in trace amounts:

- vinyl esters of fatty acids (starting material);
- acetaldehyde (formed from the vinyl alcohol portion of the vinyl fatty acid esters during the transesterification reaction); and
- p-methoxyphenol (a stabilizer added at a concentration of 20 mg/kg to the vinyl palmitate and vinyl stearate).

All residual materials, solvents and other impurities are largely removed during the purification steps.

The residual levels of vinyl fatty acid esters in several final products are summarized in Table 4. The levels of residual vinyl palmitate and vinyl stearate are measured by a validated high performance liquid chromatographic (HPLC) method with a lower limit of quantification of 1 mg/kg. The levels of vinyl laurate were determined using a GC method that has a lower limit of quantification of 10 mg/kg. The residual levels in the final products on a percentage basis are extremely low, vinyl palmitate and vinyl stearate are all under 0.0001% in their products whereas vinyl laurate are under 0.001% in its product. Considering that the sucrose esters of fatty acids are used at low levels in food products, the levels of vinyl esters of fatty acid impurities are also very low.

Table 4. Residual Levels of Vinyl Ester in Several Manufactured Lots

Material	**Residual levels** [mg/kg (%)]				
Sucrose ester of lauric acid	**MT09L001**	**MT10A001**	**MTA10A002**		
Vinyl laurate	<10 (<0.001)	<10 (<0.001)	<10 (<0.001)		
Sucrose ester of palmitic acid	**SII09F013**	**SII09F014**	**SII09G002**	**SII09G003**	**SII09G004**
Vinyl palmitate	<1 (<0.0001)	<1 (<0.0001)	<1 (<0.0001)	<1 (<0.001)	<1 (<0.0001)
Sucrose ester of stearic acid	**MT10A003**	**MT10A004**	**MT10A005**		
Vinyl stearate	<1 (0.0001)	<1 (0.0001)	<1 (0.0001)		

The levels of residual acetaldehyde in several manufactured lots of the final products are summarized in Table 5. The levels of acetaldehyde are measured using high performance liquid chromatography (HPLC) after derivatization with dinitrophenylhydrazine (DNPH) to form a UV absorbing substance, acetoaldehyde-2,4-dinitrophenylhydrazone (ADNPH). The method has been validated and the lower limit of quantification is 0.005 mg/kg. The residual levels of acetaldehyde were in general less than 0.005 mg/kg (0.000005%) in the final products.

Table 5. Residual Levels of Acetaldehyde In Several Manufactured Lots

Material	**Residual levels** [mg/kg (%)]				
Sucrose ester of lauric acid	**MT09L001**	**MT10A001**	**MT10A002**		
Acetaldehyde	<0.005 (0.000005)	<0.005 (0.000005)	<0.005 (0.000005)		
Sucrose ester of palmitic acid	**SII09F013**	**SII09F014**	**SII09G002**	**SII09G003**	**SII09G004**
Acetaldehyde	<0.005 (0.000005)	<0.005 (0.000005)	<0.005 (0.000005)	<0.005 (0.000005)	<0.005 (0.000005)
Sucrose ester of stearic acid	**MT10A003**	**MT10A004**	**MT10A005**		
Acetaldehyde	<0.005 (0.000005)	<0.005 (0.000005)	<0.005 (0.000005)		

The residual levels of p-methoxyphenol (hydroquinone monomethyl ether, MEHQ) in several manufactured lots of the final products are summarized in Table 6. The concentrations of p-methoxyphenol are determined by gas chromatography. The lower limit of quantification is 1 mg/kg. The residual levels of p-methoxyphenol were in general less than 1 mg/kg (0.0001%) in the final products. No p-methoxyphenol residues are expected in the sucrose esters of lauric acid since the stabilizer is not added to vinyl palmitate and vinyl stearate.

Table 6. Residual Levels of p-Methoxyphenol in Several Manufactured Lots

Material	**Residual levels** [mg/kg (%)]				
Sucrose ester of palmitic acid	**SII09F013**	**SII09F014**	**SII09G002**	**SII09G003**	**SII09G004**
p-methoxyphenol	<1 (0.0001)	<1 (0.0001)	<1 (0.0001)	<1 (0.0001)	<1 (0.0001)
Sucrose ester of stearic acid	**MT10A003**	**MT10A004**	**MT10A005**		
p-methoxyphenol (	<1 (0.0001)	<1 (0.0001)	<1 (0.0001)		

5. Functional use

5.1 Technological function

Sucrose monoesters of lauric, palmitic or stearic acid have higher HLB (hydrophobic-hydrophilic balance) values in the range of 18 indicating that they are efficient emulsifiers. Thus, the required level of this substance in different food preparations is relatively small. The proposed usage is an emulsifier for flavour concentrates, colour concentrates or nutraceutical products in different beverage types allowing the formulation of clear beverages.

5.2 Food categories and use levels

The uses and use levels for sucrose esters of fatty acids are not currently reported in the General Standard for Food Additives (GSFA). The proposed use of sucrose monoesters of lauric, palmitic or stearic acid allow the emulsification of flavor concentrates, color concentrates or nutraceutical products in different beverage types to allow the formulation of clear beverages.

Table 7 summarizes the new proposed food uses and use levels for sucrose esters of fatty acids based on the food category system of the GSFA of the Codex Alimentarius Commission (2007).

Table 7. Food Uses and Use Levels for Sucrose Mono Esters of Lauric, Palmitic or Stearic Acid

Food category[1]	Food use[1]		Use level (mg/kg)
01.0 Dairy products and analogues, excluding products of food category 02.0	01.1.1.1	Milk (plain)	75
	01.1.1.2	Buttermilk (plain)	75
14.0 Beverages, excluding dairy products	14.1.1.2	Table waters and soda water	220
	14.1.2.1	Fruit Juice	220
	14.1.4	Water-based flavored drinks, including "sport," "energy," or "electrolyte" drinks and particulated drinks	220
	14.1.4.1	Carbonated water-based flavored drinks	195
	14.1.4.2	Noncarbonated water-based flavored drinks including punches and ades	50
	14.2.1	Distilled spiritous beverages containing more than 15% alcohol	25
	14.1.5	Coffee, coffee substitutes, tea, herbal infusions and other hot cereal and grain beverages excluding cocoa	100

[1] Food category system (Annex B) of the GSFA of the Codex Alimentarius Commission *[CODEX STAN 192-1995 (Rev. 6-2005)] (Codex Alimentarius Commission, 2007).*

5.3 Estimated exposures

The use of sucrose monoesters of lauric, palmitic and stearic acid are restricted to formulating various beverages products based on their higher HLB values. Based on food consumption survey data from the United States (NHANES, 2003/2004 (USDA, 2009)), estimated exposures were determined and are summarized in Tables 8 and 9.

Based on the proposed uses, the estimated mean and 90th percentile all-user intake of the general population of sucrose monoesters of lauric, palmitic and stearic acid used in different beverage formulations was determined to be 2.3 mg/kg bw/day and 4.7 mg/kg bw/day.

Since other more traditional forms of sucrose esters of fatty acids are used as emulsifiers in other food types, the estimated intakes for these uses can also be determined. The estimated mean and 90th percentile all-user intake for the general population in the United States was determined to be 5.5 mg/kg bw/day and 12.2 mg/kg bw/day. Thus the intakes for the proposed beverage uses are only a small proportion of the current intakes for traditional sucrose esters of fatty acids and the combined intakes are significantly lower than the established group ADI of 30 mg/kg bw/day for sucrose monoesters of lauric, palmitic or stearic acid together with sucrose esters of fatty acids, sucroglycerides, sucrose oligoesters type I and sucrose oligoesters type II .

Table 8. Summary of the Estimated Daily Intake of Sucrose Fatty Acid Esters from All Proposed Food Categories in the U.S. by Population Group (2003-2004 NHANES Data)

Population Group	Age (years)	Percent Users (%)	Actual No. of Users	All Person		All User	
				Mean (mg)	90^{th} Percentile (mg)	Mean (mg)	90^{th} Percentile (mg)
Infants	0 to 2	75.3	700	70	146	85	160
Children	3 to 11	99.5	1,280	102	174	103	174
Female Teenagers	12 to 19	99.0	982	129	238	130	238
Male Teenagers	12 to 19	99.4	993	173	305	175	305
Female Adults	20 and up	95.8	2,039	111	239	116	245
Male Adults	20 and up	96.7	1,865	151	324	156	330
Total Population	All Ages	95.1	7,859	127	255	131	259

Table 9. Summary of the Estimated Daily Per Kilogram Body Weight Daily Intake of Sucrose Fatty Acid Esters from All Proposed Food Categories in the U.S. by Population Group (2003-2004 NHANES Data)

Population Group	Age (years)	Percent Users (%)	Actual No. of Users	All Person		All User	
				Mean (mg/kg bw)	90^{th} Percentile (mg/kg bw)	Mean (mg/kg bw)	90^{th} Percentile (mg/kg bw)
Infants	0 to 2	75.3	700	5.8	12.4	7.0	13.4
Children	3 to 11	99.5	1,280	3.9	6.8	3.9	6.8
Female Teenagers	12 to 19	99.0	982	2.2	3.9	2.2	3.9
Male Teenagers	12 to 19	99.4	993	2.6	4.5	2.7	4.5
Female Adults	20 and up	95.8	2,039	1.5	3.3	1.6	3.3
Male Adults	20 and up	96.7	1,865	1.8	3.6	1.8	3.7
Total Population	All Ages	95.1	7,859	2.2	4.6	2.3	4.7

6. Reactions and fate in foods

Under conditions of use in fruit flavored beverages, that have pH in the range of 3.8 - 5.0, it is expected that some hydrolysis of the sucrose fatty acid esters may occur, resulting in the formation of small amounts of free sucrose or fatty acids. Sucrose may also hydrolyze further into glucose and fructose.

A number of surrogate stability studies have been reported for sucrose monolaurate and sucrose monostearate. Sucrose monolaurate (9.6 mM) in buffer solutions at pH values 2.1, 2.5, 3.0, 4.06, 5.08, 5.80, 6.80, 7.20 and 9.3 were heated to 100°C for 20 hours and analyzed for free lauric acid over time. Maximum stability occurred between pH 4 to 5 where approximately 6.7% hydrolysis occurred after 20 hours at 100°C. Below critical micelle concentration, the degradation kinetics were first order, while at concentrations above critical micelle concentration the degradation reaction were not first order. The release of lauric acid allowed formation and interactions between micelles protecting the sucrose monolaurate from acid hydrolysis. Thus, at 25°C, no considerable hydrolysis would take place over the course of several weeks (Anderson and Polack, 1968).

7. References

Anderson, R.A. and Polack, A.E. 1968. The stability of sucrose monolaurate: rate of formation of lauric acid. J Pharm Pharmac 20:249-254.