

Flavor Properties of FEMA GRAS List 26 Flavor Chemicals

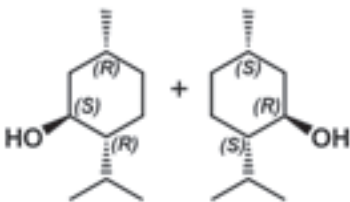
A preliminary assessment.

John Leffingwell and Diane Leffingwell, Leffingwell & Associates

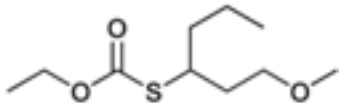
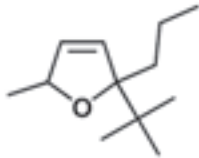
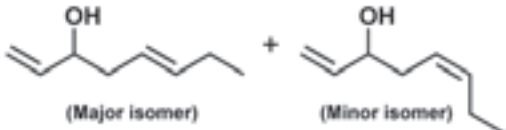
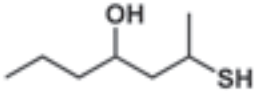
The Flavor and Extract Manufacturers Association released its GRAS 26 list in 2013. Here, the authors present a table of the ingredients, descriptions and structures, where available (T-1).

—Editor

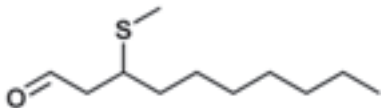
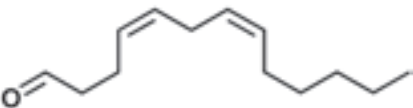
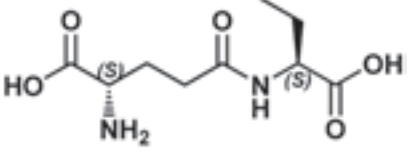
T-1. FEMA GRAS 26 descriptions and structures

FEMA#	CAS#	Name	Description	Structure
4728	57817-89-7	Glucosyl steviol glycosides; stevia extract, enzymatically modified	Natural low calorie sweetener and flavor enhancer. Glucosyl steviol glycosides are a complex mixture of glycosides prepared by enzymatically modifying stevia extract to increase/change the degree of glycosylation. In United States Patent 8318459 (Nov. 27, 2012) by Avetik Markosyan titled "Glucosyl stevia composition" (assigned to PureCircle USA), it is demonstrated that improved sweetness profiles can be achieved. In WIPO Patent Application W02012128775 by Siddhartha Purkayastha, "Glucosylated Steviol Glycoside Composition as a Taste and Flavor Enhancer" (assigned to PureCircle USA), and WIPO Patent Application W02012129451 by Siddhartha Purkayastha, "Glucosylated Steviol Glycoside Composition as a Taste and Flavor Modifier" (assigned to PureCircle USA), the use of the materials in modifying the flavor profiles of various products is described.	Not available. Complex mixture of stevia extract glucosides.
4729	3623-52-7	Isomenthol; dl-isomenthol; (±)-isomenthol	(-)-Menthol has considerably more cooling power than dl-isomenthol alone. dl-Isomenthol features a somewhat musty, woody camphoric odor. However, in U.S. Patent 8496950 (July 30, 2013) by Klaus Sorge, Hubert Loges, Arnold Machinek, Ulrike Simchen and Horst Surburg, "Mixture	

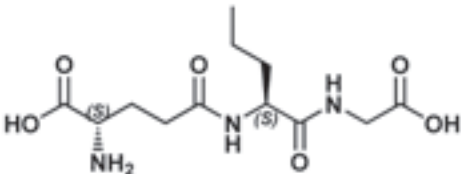
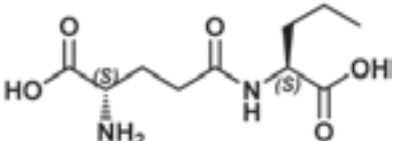
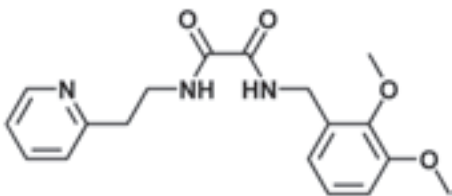
T-1. FEMA GRAS 26 descriptions and structures (Cont.)

FEMA#	CAS#	Name	Description	Structure
			Containing Menthol," assigned to Symrise, the use of dl-isomenthol in various menthol mixtures has been shown to lower their melting point. In addition, the organoleptic perception is acceptable or improved at the levels used.	
4730	1241905-19-0	Ethyl S-(1-methoxyhexan-3-yl)carbonothioate; O-ethyl S-(1-methoxyhexan-3-yl) carbonothioate	Flavor description: Sulfury, blackcurrant, tropical, roasted coffee; effective in coffee. Odor description: Mushroom, herbaceous, slightly cacao connotation. This material is the subject of WIPO Patent Application WO/2010/115920, "Carbonothioates as Flavours and Fragrances" (10/14/2010) by Klaus Gassenmeier, assigned to Givaudan.	
4731	871465-49-5	Cassyrane; ^a 2-tert-butyl-5-methyl-2-propyl-2,5-dihydrofuran	In U.S. Patent 7,632,790 (Dec. 15, 2009) by Philip Kraft and assigned to Givaudan, this material's odor description is as follows: blackcurrant, natural, rich, eucalyptus buds, anise, buchu leaves, slightly green. ^b	
4732	83861-74-9	1,5-Octadien-3-ol; octa-1,5-dien-3-ol	Mixture of E/Z stereoisomers with 60–90% (E). The material possesses earthy, mushroom, green, geranium leaf and marine notes. Boelens (PMP 2001, "Database of Perfumery Materials & Performance") indicates: dusty, somewhat earthy, mushroom-like odor. Delort et al. have described (Z)-1,5-octadien-3-ol's orthonasal odor as green, marine, slightly mushroom and strong, and its retronasal odor (10 ppm) as floral, green, geranium leaf, crustaceous, mushroom and metallic. ¹	
4733	1006684-20-3	2-Mercapto-4-heptanol	Flavor description: fruity, tropical, guava, watercress, vegetal (at 0.5 ppm in 5% sugar solution). ² The flavor description is for the diastereomeric mixture.	

T-1. FEMA GRAS 26 descriptions and structures (Cont.)

FEMA#	CAS#	Name	Description	Structure
4734	1256932-15-6	3-(Methylthio) decanal	At the time of this writing the authors have no definitive information on the flavor of this material. Based on the chemical structure, the authors anticipate that the organoleptic character would approximate "roasted, fatty, aldehydic." The ingredient primarily finds use in savory, meat and fish flavors.	
4735	13552-95-9	(4Z,7Z)-Tridecadienal	(4Z,7Z)-Tridecadienal is a fatty flavor aldehyde originally discovered by Lever Bros. to be useful in fatty, savory flavors. In Great Britain Patent 1,034,352, Dutch Pat. No. 139,102 and Swiss Pat No. 471545, it is reported that <i>cis</i> -4-decenal, <i>cis,cis</i> -4,7-tridecadienal and other polyunsaturated aldehydes containing 11–17 carbon atoms are suitable for imparting a savory aroma that enhances chicken meat flavor to foodstuffs. In Japanese Patent JP2012034662 (Feb. 23, 2012) by Tsukasa Saito et al., "Dried Fish Flavor Improving Agent" (assigned to T. Hasegawa), the use of 2,4,7-tridecatrienal and/or 4,7-tridecadienal for producing dried fish flavors (specifically, dried bonito) is disclosed. At low levels they can also impart umami effects.	
4738	16869-42-4	L-γ-Glutamyl-L-2-aminobutyric acid; γ-glu-abu	This is a kokumi-imparting agent. U.S. Patent Application 20120034364 (Feb. 9, 2012) by Fumie Futaki et al., "Use of Peptides for Imparting Kokumi," describes a substance that provides a kokumi-imparting agent consisting of γ-glu-abu (L-γ-glutamyl-L-2-amino-butyric acid). The kokumi-imparting agent of the present invention, or γ-glu-abu, can be used in combination with at least one additional ingredient for seasonings selected from the group consisting of amino acids such as sodium glutamate (MSG), nucleic acids such as inosine monophosphate (IMP), inorganic salts such as sodium chloride, organic acids such as citric acid,	

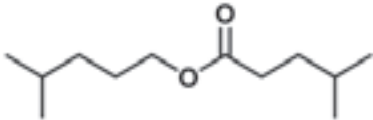
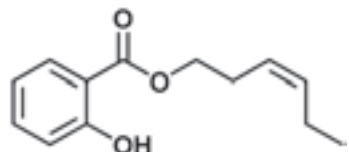
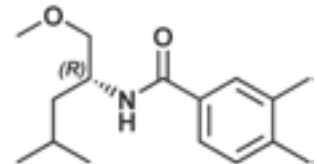
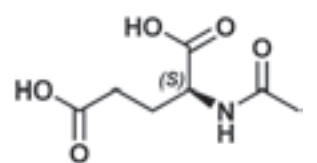

T-1. FEMA GRAS 26 descriptions and structures (Cont.)

FEMA#	CAS#	Name	Description	Structure
			and various types of yeast extracts to provide a favorable seasoning composition that is improved in its kokumi, as compared to those obtained by the use of such additional ingredients for seasonings individually.	
4739	38837-71-7	Glutamyl-norvalyl-glycine; N-(N-L-γ-glutamyl-L-norvalyl)-glycine; L-glutamyl-L-norvalyl-glycine; γ-glu-nva-gly	This is a kokumi flavor enhancer. WIPO Patent Application WO2011081186 (July 7, 2011) by Takashi Miyaki et al., "Flavor-Enriching Agent," discloses that γ-glu-nva-gly (L-γ-glutamyl-L-norvaline-glycine) exhibits a potent flavor-enriching action, particularly with respect to middle tastes, and exhibits an improved stability.	
4740	71133-09-0	Glutamyl-norvaline; L-γ-glutamyl-L-norvaline N-(N-L-γ-glutamyl)-L-norvaline; L-glutamyl-L-norvaline; γ-glu-nva	This material is a kokumi flavor enhancer. γ-Glu-nva (L-γ-glutamyl-L-norvaline) is the subject of U.S. Patent 8541379 (Sept. 24, 2013) by Takashi Miyaki et al., "Kokumi-imparting agent" (assigned to Ajinomoto). The patent provides examples of the kokumi effect of L-glutamyl-L-norvaline wherein the intensity of the kokumi-imparting activity observed for each test compound was determined as a value observed when blending 0.00001–0.5 g/dL of the corresponding test compound with distilled water containing sodium glutamate (0.05 g/dL), inosinic acid monophosphate (0.05 g/dL) and sodium chloride (0.5 g/dL). The kokumi effect was effective at a dose level of 0.0001 g/dL, which was a significantly lower dose level than a number of other kokumi compounds tested.	
4741	851670-40-1	N-(2,3-Dimethoxybenzyl)-N'-(2-(pyridin-2-yl)ethyl)oxalamide; N1-(2,3-dimethoxybenzyl)-N2-(2-(pyridin-2-yl)ethyl)oxalamide	This savory material is an umami flavor enhancer. It is disclosed and identified as an umami compound in U.S. Patent 7476399 (01/13/2009), "Flavors, flavor modifiers, tastants, taste enhancers, umami or sweet tastants, and/or enhancers and use thereof," by Catherine Tachdjian et al. (assigned to Senomyx).	

T-1. FEMA GRAS 26 descriptions and structures (Cont.)

FEMA#	CAS#	Name	Description	Structure
4742	917750-72-2	1-(2-Hydroxy-4-methylcyclohexyl) ethanone	In U.S. Patent 8,071,531 (Dec. 6, 2011) by Takashi Aida and Kenya Ishida, "Flavor and fragrance composition" (assigned to Takasago), this material is described as having an acetophenone-like odor with sweetness. In aqueous solution, the authors note that the material provides a "cool and refreshing feeling equivalent to 10 ppm of menthol at a concentration of 50 ppm; appearance of refreshing feeling is relatively rapid with clear refreshing feeling without unpleasant taste." The material has a synergetic effect with menthol. A 70:30 mixture of l-menthol and (1R,2R,4R)-1-(2-hydroxy-4-methylcyclohexyl)ethanone showed about 40% stronger cool and refreshing feeling than that of menthol alone.	
4745	62439-41-2	(±)-6-Methoxy-2,6-dimethylheptanal; methoxymelonal	This material has citrus, floral and fruity notes with a watery melon character. It was first reported in U.S. Patent 4311617 (Jan. 19, 1982) by Hifzur R. Ansari et al., "Perfumery compositions." It has long been used in fragrances. Michael Zviely reports it has "a light floral odor, slightly fruity note with a watery citrus character. It is fresh, herbaceous and slightly fruity with melon connotations." ³	
4746	68973-20-6	3,5-Undecadien-2-one	The odor of this material is described by Sungim Im et al. as "fatty, fried" by GC-O. ⁴ 3,5-Undecadien-2-one was also described as "fatty, fried" by H.T. Badings, as referenced by David A. Forss. ⁵	
4747	91212-78-1	(±)-2,5-Undecadien-1-ol; undeca-2,5-dien-1-ol	The authors are unfamiliar with this material, but by analogy anticipate it to have a somewhat fatty, waxy character. The related 2,4-undecadien-1-ol has been described by both Bedoukian and Boelens as a "mild, fatty odor." (Z,Z)-2,5-Undecadien-1-ol is found in noni (<i>Morinda citrifolia</i> L.).	
4748	54717-17-8	Triethylthialdine; 2,4,6-triethyl-1,3,5-dithiazinane; 5,6-dihydro-2,4,6-triethyl-4H-1,3,5-dithiazine	This material's profile is sulfurous, fried onion, leek, meaty, savory, seafood. Boelens (PMP 2001, "Database of Perfumery Materials & Performance") indicates that the material is "narcotic, sulfurous- and amine-like; seafood note." Literature from Treatt indicates	

T-1. FEMA GRAS 26 descriptions and structures (Cont.)

FEMA#	CAS#	Name	Description	Structure
			that the material is sulfurous, savory and "cooked leek." The ingredient can be used in flavors for oils and fats at 0.35–3.5 ppm; in meat and dairy flavors for snack foods and sauces at 3–6 ppm; and in soups and seasonings at 4–8 ppm. The material is also described as a powerful "fried onion" note. It is also described as weak raw pumpkin, white part of allium plants (at pH 7.3) and green, leek at lower pH. ⁶	
4749	35852-42-7	4-Methylpentyl 4-methylpentanoate; 4-methylpentyl 4-methylvalerate; isohexyl isohexanoate	This material is sweet, fruity, waxy, soapy and slightly herbal. It is considered sensorially relevant to capsicum peppers and is primarily used in fruit flavors	
4750	65405-77-8	<i>cis</i> -3-Hexenyl salicylate; (<i>Z</i>)-3-hexenyl salicylate; (<i>Z</i>)-hex-3-enyl salicylate	This material is sweet, green, floral, woody and balsamic. It is used as a modifier in floral and fruit flavors.	
4751	851669-60-8	(<i>R</i>)-N-(1-Methoxy-4-methylpentan-2-yl)-3,4-dimethylbenzamide	This savory material is an umami flavor enhancer. It is disclosed and identified as an umami compound in U.S. Patent 7476399 (01/13/2009), "Flavors, flavor modifiers, tastants, taste enhancers, umami or sweet tastants, and/or enhancers and use thereof," by Catherine Tachdjian et al. (assigned to Senomyx).	
4752	1188-37-0	Acetyl glutamate; N-acetyl-L-glutamate; N-acetyl-L-glutamic acid; α-(N-acetyl)-L-glutamic acid	This material is an umami-like flavor enhancer. In WIPO Patent Application WO2013010991 (Jan. 24, 2013) by Xiaogen Yang et al., "Flavour Modifying Compounds" (assigned to Givaudan) it is disclosed that N-acetyl glutamic acid can modify the taste or flavor, in particular the salt taste, umami taste, or savory flavor of a flavor composition or consumable product.	
4753	504-63-2	1,3-Propanediol; 1,3-Propylene glycol; Zemea propanediol ^c	This is a certified natural product replacement for 1,2-propylene glycol; it can be used to replace glycols such as propylene glycol (1,2-propanediol), butylene glycol (1,3-/1,4-butanediol) and glycerin.	

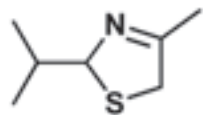
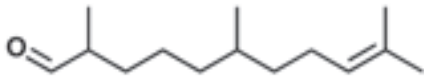
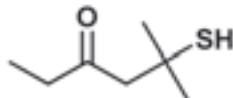
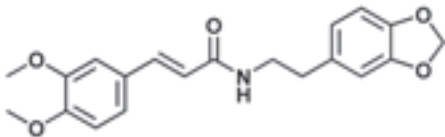
T-1. FEMA GRAS 26 descriptions and structures (Cont.)

FEMA#	CAS#	Name	Description	Structure
4758	20921-04-4	Ethyl melilotate; Ethyl 3-(2-hydroxyphenyl) propanoate; ethyl 3-(2-hydroxyphenyl) propionate	This material adds sweetness, extends vanilla character and contributes sweet-cream-vanilla notes. In WIPO Patent Application WO2013000595 (Jan. 3, 2013) by Estelle Delort and Erik Decorzant, "Flavoring Compound" (assigned to Firmenich), ethyl 3-(2-hydroxyphenyl) propanoate is disclosed as a flavoring ingredient that imparts or reinforces a coumarin and/or vanilla tonality.	
4759	16510-27-3	Toscanol; ^d 1-(cyclopropylmethyl)-4-methoxybenzene; 1-cyclopropylmethyl-4-methoxybenzene; p-(cyclopropylmethyl) anisole	This material is described as strong anisic, estragole, anethole, sassafras and cresolic. Givaudan indicates Toscanol's odor as: Anisic, green, liqueur-like and herbaceous. It can be used for a powerful and linear anisic, sweet-spicy note of estragole (methyl chavicol), licorice and sassafras oil character with a touch of saffron, myrtle, opopanax and carvi seeds. Toscanol can be used in all kinds of accords to add anisic agrestic and aromatic character. See also: U.S. Patent 7704942 (April 27, 2010), "Fragrance and flavour compositions," by Andreas Goeke (assigned to Givaudan).	
4760	53626-94-1	S-Prenyl thioisobutyrate; S-(3-methylbut-2-enyl) 2-methylpropanethioate	Boelens (PMP 2001, "Database of Perfumery Materials & Performance") indicates that the material is sulfurous, fruity, tropical fruit connotation, durian and passion fruit odor. Its primary use is probably vegetable, savory, tropical fruit, and pineapple flavors. It is found in <i>Agathosma</i> oils related to buchu.	
4761	75631-91-3	S-Prenyl thioisovalerate; S-3-methylbut-2-enyl 3-methylbutanethioate; S-prenyl thioisopentanoate; S-(3-methylbut-2-en-1-yl) 3-methylbutanethioate	This material possesses sulfurous, fruity, tropical fruit connotations, durian and passion fruit notes. Its primary use is probably vegetable, savory, tropical fruit, and pineapple flavors. It is found in <i>Agathosma</i> oils related to buchu.	
4762	580-72-3	(-)-Matairesinol; (8R,8'R)-(-)-matairesinol; (3R,4R)-dihydro-3,4-bis[(4-hydroxy-3-methoxyphenyl)methyl]-2(3H)-furanone; (3R,4R)-3,4-bis[(4-hydroxy-3-methoxyphenyl)methyl] oxolan-2-one	This material reduces bitterness and astringency. In European Patent Application EP2517574 (Oct. 31, 2012) by Michael Backes et al., "Specific vanillyl lignanes and their use as taste enhancers" (assigned to Symrise), the use of (-)-matairesinol has been shown to reduce both bitter impressions and astringency at levels of about 25–100 ppm.	

T-1. FEMA GRAS 26 descriptions and structures (Cont.)

FEMA#	CAS#	Name	Description	Structure
4763	57817-89-7	Stevioside; steviosin; (4, α)-13-[(2-O- β -D-glucopyranosyl- α -D-glucopyranosyl)oxy] kaur-16-en-18-oic acid β -D-glucopyranosyl ester	<p>This material is a natural low-calorie sweetener. Steviol glycosides are responsible for the sweet taste of the leaves of the stevia plant (<i>Stevia rebaudiana</i> Bertoni). These compounds range in sweetness from 40 to 300 times sweeter than sucrose.</p> <p>The four major steviol glycosides found in the stevia plant tissue are:</p> <ul style="list-style-type: none"> • 5–10% stevioside (250–300x of sugar) • 2–4% rebaudioside A (most sweet and least bitter; 350–450x of sugar) • 1–2% rebaudioside C • 0.5%–1% dulcoside A 	
4764	50297-39-7	1-(2,4-Dihydroxyphenyl)-3-(3-hydroxy-4-methoxyphenyl)propan-1-one	<p>This material is a sweetness enhancer and bitterness reducer. In U.S. Patent Application 20080113073 (May 15, 2008) by Jakob Ley et al., "Hydroxydeoxybenzoins and the Use Thereof to Mask a Bitter Taste," this material demonstrated enhanced sweetness of sucrose and reduced bitterness of caffeine.</p>	
4765	1367348-37-5	Ethyl 5-(formyloxy) decanoate; ethyl 5-formyloxydecanoate	<p>This material is a δ-decalactone precursor; it forms δ-decalactone when heated or under enzymatic conditions. It is dairy-like, and so is useful in dairy flavors, or wherever δ-decalactone might be employed.</p>	
4766	1160112-20-8	3-[3-(2-Isopropyl-5-methyl-cyclohexyl)ureido]butyric acid ethyl ester; ethyl 3-(3-(menthyl)ureido)butyrate; ethyl 3-(3-(2-isopropyl-5-methylcyclohexyl)ureido)butanoate	<p>This material is salty, metallic and umami-like. U.S. Patent Application 20090311401 (Dec. 17, 2009) by Jakob Peter Ley et al., "Neo-Menthyl Derivatives as Flavor Materials" (assigned to Symrise), discloses a series of ureas, thioureas, carbamates, thiocarbamates and guanidines based on the neomenthyl structure as flavor materials or flavor material mixtures for producing, imparting, modifying and/or enhancing savory flavor notes. The racemic mixture of 3-[3-((1S,2S,5R)-2-isopropyl-5-methyl-cyclohexyl)ureido]-butyric acid ethyl ester (compound 7)</p>	

T-1. FEMA GRAS 26 descriptions and structures (Cont.)

FEMA#	CAS#	Name	Description	Structure
			and 3-[3-((1R,2R,5S)-2-isopropyl-5-methyl-cyclohexyl)-ureido]-butyric acid ethyl ester (compound 8) had a flavor profile of: bitter, salty, metallic and umami.	
4767	67936-13-4	2-Isopropyl-4-methyl-3-thiazoline; 2-isopropyl-4-methyl-2,5-dihydrothiazole; 2,5-dihydro-2-isopropyl-4-methylthiazole	This is a flavor enhancer for fruit flavors, brown flavors and savory flavors. In European Patent Application EP2289351 (Mach 2, 2011) by Kathryn A. Bardsley et al., "Use of thiazoline compounds in flavor applications" (assigned to IFF), the flavor use of 2-isopropyl-4-methyl-3-thiazoline is disclosed. Its detection threshold is 10 ppb (slightly fruity, tropical, peach, berry). At 50 ppm, it is described as rubber, phenolic and mushroom.	
4768	141-13-9	Adoxal; ^e 2,6,10-trimethyl-9-undecenal	This material is fresh, aldehydic, powerful, floral, rosy and ozonic-marine. Givaudan indicates: "Olfactive note—fresh, aldehydic, powerful, floral, rosy, marine. Description—Adoxal blends extremely well with floral notes such as muguet and cyclamen, as well as with fruity and woody compositions. It can also be seen as having a typical 'fresh linen' odor and a natural, ozonic aspect."	
4769	851768-51-9	5-Mercapto-5-methyl-3-hexanone; Sauvignone 100 ^f	This material can be described as sparkling citrus, grape, fruity and watery, with tropical notes. Takasago indicates: "Odor Description: Sparkling citrus, grape. Very effective in watery applications where traces provide interesting effects, obviously in fruity notes."	
4773	125187-30-6	Rubescenamine; (E)-N-[2-(1,3-benzodioxol-5-yl)ethyl]-3-(3,4-dimethoxyphenyl)prop-2-enamide	This material is an umami flavor enhancer. In U.S. Patent Application 20120308703 (Dec. 6, 2012) by Jakob Peter Ley et al., "Cinnamides as Savory Flavorings" (assigned to Symrise), rubescenamine (along with a number of structurally similar compounds) is disclosed as an excellent savory flavor ingredient. Rubescenamine at 5 mg/kg test concentration is characterized by an umami taste that is very similar to that of monosodium glutamate (MSG), which above all enhances the mouthfeel, meaty character and mouth-watering effect significantly, without tasting unpleasantly sweet.	

T-1. FEMA GRAS 26 descriptions and structures (Cont.)

FEMA#	CAS#	Name	Description	Structure
4774	1359963-68-0	4-Amino-5-(3-(isopropylamino)-2,2-dimethyl-3-oxopropoxy)-2-methylquinoline-3-carboxylic acid;	This sweetness enhancer/modifier is covered by the claims in Senomyx's U.S. Patent Application 20110245353 (Oct. 6, 2011), "Sweet Flavor Modifier," and specifically mentioned in Senomyx's U.S. Patent Application 20120041078 (Feb. 16, 2012), "Method of Improving Stability of Sweet Enhancer and Composition Containing Stabilized Sweet Enhancer."	
4775	67801-20-1	Ebanol; ^g 3-methyl-5-(2,2,3-trimethylcyclopent-3-en-1-yl)pent-4-en-2-ol	Givaudan indicates: "Olfactive note: Sandalwood, musk aspect powerful. Description: Ebanol has a very rich, natural sandalwood odor. It is powerful and intense, bringing volume and elegance to woody accords and a diffusive sandalwood effect to compositions. Ebanol is highly substantive on all supports." ^h	
4776	198404-98-7	Javanol; ⁱ (1-methyl-2-(1,2,2-trimethylbicyclo[3.1.0]-hex-3-ylmethyl) cyclopropyl) methanol (mixture of diastereoisomers)	This material is one of the most powerful and best of the sandalwood replacements. Givaudan indicates: "Olfactive note: Sandalwood, creamy, rosy, powerful. Description: Javanol is a new-generation sandalwood molecule with unprecedented power and substantivity. It has a rich, natural, creamy sandalwood note like β-santalol. With its exceptional low threshold, it is approximately 8x more effective in wash tests on a weight basis than the most powerful known product."	

^gCassyrane is a registered trademark of Givaudan S.A.

^hDescriptions of the enantiomers can be found at www.leffingwell.com/chirality/cassyrane.htm

^cZemeais a registered trademark of DuPont Tate & Lyle Bio Products Co., LLC

^dToscanol is a registered trademark of Givaudan S.A.

^eAdoxal is a trade name of Givaudan S.A.

^fSauvignone 100 is a trade name of Takasago

^gEbanol is a registered trademark of Givaudan S.A.

^hThe enantiomers of Ebanol are described at: www.leffingwell.com/chirality/ebanol.htm

ⁱJavanol is a registered trademark of Givaudan S.A.

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