

Compositions with Aroma and Methods Thereof

Technical Field

- 5 The present disclosure concerns, in general terms, to compositions with aroma and the methods thereof.

Background

- 10 Fragrances are considered normal components of our everyday lives. Many people wear a fragrance in order to feel good. Studies have shown that there is a connection between scent and emotion as well as between scent and memory. Studies have also shown that some fragrances can alter moods and even alleviate anxiety and stress.

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- Perfume is a mixture of fragrant essential oils or aroma compounds (fragrances), fixatives and solvents, usually in liquid form, used to give the human body, animals, food, objects, and living-spaces an agreeable scent. Perfumes can be defined as substances that emit and diffuse a pleasant and
- 20 fragrant odour. They consist of manmade mixtures of aromatic chemicals and essential oils. Until the nineteenth century perfumes were usually composed of natural aromatic oils. Nowadays, most perfumes are synthetic and may contain many components. This is in part due to natural fragrance being expensive to produce and limited in their availability.

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- Perfumes can be classified according to the note type they provide, i.e., according to the fragrance type. The different notes may be floral, citrus, fruity, green, woody, oriental, spice, animal, leather, etc. These notes may be categorised within a fragrance wheel chart, which separates fragrances into four
- 30 main groups (floral, fresh, woody and oriental) and further sub-divide them into 14 different families and establishes the relationships amongst them.

Another aspect of perfumes is how long the scent persists on the body. In

general, there are three main notes in a perfume, with different persistence. The top notes are responsible for the first impression, which lasts from a couple of minutes to approximately an hour, and are generated by high-volatility fragrance chemicals. The middle notes, composed by medium-volatility
5 fragrance chemicals, play the most important role in a perfume, because they are responsible of the identity of the perfume. Finally, the base notes can last for more than 6 h and are composed by low-volatility chemicals. The balance amongst all these notes enables perfumes to be more or less persistent. Adding fragrance modifiers and fixatives can help to increase perfume persistence.

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The global perfume market size was USD 29.8 billion in 2020. The market is projected to grow from USD 30.6 billion in 2021 to USD 43.2 billion in 2028 at a CAGR of 5.0% in the 2021-2028 period.

15 While there are more than 2500 fragrances which can be used in a plethora of combinations to provide a wide range of scents, some of these fragrances are very expensive and are not ideal for large scale manufacturing. Many of these chemicals are also classified as allergens, hormone disruptors, asthma triggers, neurotoxins and carcinogens; in other words fragrances are highly toxic.
20 Accordingly, there is a need for safer fragrances.

There is a constant need for new aroma component in order to satisfy a multitude of applications. In particular, the compounds should have certain properties in order for them to be functional as an aroma component for use in
25 cosmetics, cleaning and/or food applications. For example, the compounds by themselves should have good olfactory properties, should also be relatively easy to prepare, have a certain level of purity, is non-toxic, is chemically and physically stable and can synergistically interact with other aroma compounds to provide a desirable sensory profile.

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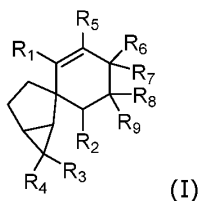
However, since even small changes in chemical structure bring about massive changes in the sensory properties, the search for compounds with acceptable sensory properties is extremely difficult.

It would be desirable to overcome or ameliorate at least one of the above-described problems.

5 Summary

The present disclosure is predicated on the understanding that some terpene compounds may have a desirable odour. As terpene compounds are naturally occurring, and may be found in plants and animals, they are generally deemed
 10 to be safe to humans. Accordingly, terpene compounds may be used as an aroma compound to impart an aroma which is safe to humans.

The present disclosure provides a composition, comprising:
 a compound of Formula (I) or a salt, solvate or stereoisomer thereof:



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wherein

R₁, R₂, R₃ and R₄ are independently selected from H, oxo, optionally substituted alkyl, optionally substituted alkenyl; and

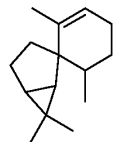
R₅, R₆, R₇, R₈ and R₉ are independently selected from H, oxo, optionally
 20 substituted alkyl, optionally substituted alkenyl;

wherein the compound of Formula (I) is characterised by a concentration of at least 80 ppm relative to the composition.

In some embodiments, R₁, R₂, R₃ and R₄ are independently optionally
 25 substituted C₁-C₄ alkyl.

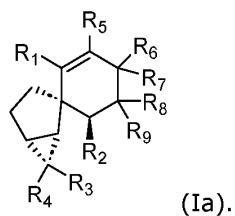
In some embodiments, R₅, R₆, R₇, R₈ and R₉ are independently selected from H, or optionally substituted C₁-C₄ alkyl.

In some embodiments, the compound of Formula (I) is

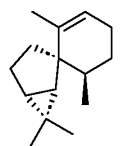


In some embodiments, the compound of Formula (I) is a compound of Formula

5 (Ia):



In some embodiments, the compound of Formula (I) is



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In some embodiments, the compound of Formula (I) is characterised by a concentration of at least 100 ppm relative to the composition.

In some embodiments, the compound of Formula (I) is characterised by a woody

15 and/or earthy scent.

In some embodiments, the composition further comprises 9-aristolene.

In some embodiments, the 9-aristolene is characterised by a concentration of

20 at least 20 ppm relative to the composition.

In some embodiments, the composition further comprises 1-aristolene.

In some embodiments, the 1-aristolene is characterised by a concentration of less than 20 ppm relative to the composition.

5 In some embodiments, the composition is characterised by a ratio of the compound of Formula (I) to 9-aristolene and 1-aristolene of about 2:1 to about 6:1.

In some embodiments, the composition is characterised by a woody, earthy and medicinal scent.

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In some embodiments, the composition further comprises another aroma chemical.

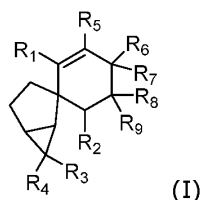
In some embodiments, the composition further comprises at least one carrier.

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The present disclosure also provides a method of formulating a composition, comprising:

adding a compound of Formula (I) or a salt, solvate or stereoisomer thereof to the composition:

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wherein

R₁, R₂, R₃ and R₄ are independently selected from H, oxo, optionally substituted alkyl, optionally substituted alkenyl; and

25 R₅, R₆, R₇, R₈ and R₉ are independently selected from H, oxo, optionally substituted alkyl, optionally substituted alkenyl;

wherein the compound of Formula (I) is characterised by a concentration of at least 80 ppm relative to the composition.

The present disclosure also provides a method of providing an aroma to a

composition, comprising a step of adding a compound of Formula (I) to the composition, wherein the compound of Formula (I) is characterised by a concentration of at least 80 ppm relative to the composition.

- 5 The present disclosure also provides a use of a compound of Formula (I) to impart an aroma, wherein the compound of Formula (I) is added such that its final concentration is at least 80 ppm.

Brief description of the drawings

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Embodiments of the present invention will now be described, by way of non-limiting example, with reference to the drawings in which:

Figure 1 shows GC-MS detection of the terpene products of the clade 5 enzymes LdSTS7 and LdSTS11. (A) Total ion chromatograms of the fermentation products of E. coli overexpressing LdSTS7 and LdSTS11, showing a major product 1 and two other minor products (2 & 3). (B) GC-MS trace of the main compound 1 produced by LdSTS7.

Figure 2 shows (A) Numbering nomenclature for compound (1), 9-aristolene (2), and 1-aristolene (3) used in NMR analysis. (B) Structure elucidation process for compound 1. (C) Observed key HMBC correlations for 1. (D) Observed key NOE correlations for 1.

Figure 3 shows mass spectrum of the fragrances using a DB-5 column.

Figure 4 shows mass spectrum of the fragrances using a wax column.

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Detailed description

"Alkyl" refers to monovalent alkyl groups which may be straight chained or branched and preferably have from 1 to 10 carbon atoms or more preferably 1 to 6 carbon atoms. Examples of such alkyl groups include methyl, ethyl, n-propyl, iso-propyl, n-butyl, iso-butyl, n-hexyl, and the like.

"Alkenyl" refers to a monovalent alkenyl group which may be straight chained or branched and preferably have from 2 to 10 carbon atoms and more preferably

2 to 6 carbon atoms and have at least 1 and preferably from 1-2, carbon to carbon, double bonds. Examples include ethenyl ($-\text{CH}=\text{CH}_2$), n-propenyl ($-\text{CH}_2\text{CH}=\text{CH}_2$), iso-propenyl ($-\text{C}(\text{CH}_3)=\text{CH}_2$), but-2-enyl ($-\text{CH}_2\text{CH}=\text{CHCH}_3$), and the like.

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"Alkoxy" refers to the group alkyl-O- where the alkyl group is as described above. Examples include, methoxy, ethoxy, n-propoxy, iso-propoxy, n-butoxy, tert-butoxy, sec-butoxy, n-pentoxy, n-hexoxy, 1,2-dimethylbutoxy, and the like.

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"Halo" or "halogen" refers to fluoro, chloro, bromo and iodo.

"Oxo/hydroxy" refers to groups $=\text{O}$, $\text{HO}-$.

15 "Amino" refers to the group $-\text{NR}^1\text{R}^2$ where each R is independently hydrogen, alkyl, cycloalkyl, aryl, heteroaryl, and heterocyclyl and where each of alkyl, cycloalkyl, aryl, heteroaryl and heterocyclyl is as described herein.

In this specification "optionally substituted" is taken to mean that a group may
20 or may not be further substituted or fused (so as to form a condensed polycyclic group) with one or more groups selected from hydroxyl, acyl, alkyl, alkoxy, alkenyl, alkenyloxy, alkynyl, alkynyloxy, amino, aminoacyl, thio, arylalkyl, arylalkoxy, aryl, aryloxy, carboxyl, acylamino, cyano, halogen, nitro, phosphono, sulfo, phosphorylamino, phosphinyl, heteroaryl, heteroarylalkyl,
25 heteroaryloxy, heterocyclyl, heterocyclylalkyl, heterocyclyoxy, oxyacyl, oxime, oxime ether, hydrazone, oxyacylamino, oxysulfonylamino, aminoacyloxy, trihalomethyl, trialkylsilyl, pentafluoroethyl, trifluoromethoxy, difluoromethoxy, trifluoromethanethio, trifluoroethenyl, mono- and di-alkylamino, mono- and di-(substituted alkyl)amino, mono- and di-arylamino, mono- and di-heteroarylamino, mono- and di-heterocyclyl amino, and unsymmetric di-
30 substituted amines having different substituents selected from alkyl, aryl, heteroaryl and heterocyclyl, and the like, and may also include a bond to a solid support material, (for example, substituted onto a polymer resin). For instance,

an "optionally substituted amino" group may include amino acid and peptide residues.

The term "aroma" refers to a sensory property and may comprise an odour
5 and/or a flavour.

The term "aroma compound" refers to a substance which is used to obtain a sensory or organoleptic (used interchangeably herein) impression and comprises its use to obtain an olfactory and/or a flavor impression. The term
10 "olfactory impression" denotes an odor impression without any positive or negative judgement, while the term "scent impression" or "fragrance impression" or "aroma impression" (used interchangeably herein) as used herein is connected to an odour which is generally felt as pleasant. A flavour induces a taste impression.

15 Notes in perfumery are descriptors of scents that can be sensed upon the application of a perfume. Notes are separated into three classes: top/head notes, middle/heart notes, and base notes; which denote groups of scents which can be sensed with respect to the time after the application of a perfume. These
20 notes are created with knowledge of the evaporation process and intended use of the perfume. The presence of one note may alter the perception of another—for instance, the presence of certain base or heart notes will alter the scent perceived when the top notes are strongest, and likewise the scent of base notes in the dry-down will often be altered depending on the smells of the heart notes.

25 Fragrances may be listed in order of volatility and grouped under respective evaporation coefficients (perfume notes) that range from 1 to 100. Top notes may have an evaporation coefficient of 1 to 14 (most volatile), middle notes of 15 to 60, and base notes of 61 to 100 (least volatile).

30 Top notes are also called the head notes. They are perceived immediately upon application of a perfume. Top notes may consist of small, light molecules that evaporate quickly. They form a person's initial impression of a perfume and thus

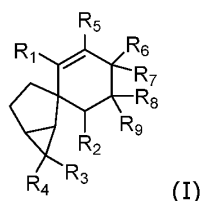
are very important in the selling of the product. The scents of this note class are usually described as "fresh", "assertive" or "sharp". The compounds that contribute to top notes are strong in scent, very volatile, and evaporate quickly. Although not as saliently perceived, the heart and base-notes contribute much
5 to the scent in the top notes. Citrus and ginger scents are common top notes.

Middle notes are also called the "heart notes". The middle notes are the scent of a perfume that emerges just before the top notes dissipate. The middle note compounds form the "heart" or main body of a perfume and emerge in the
10 middle of the perfume's dispersion process. They serve to mask the often unpleasant initial impression of base notes, which become more pleasant with time. The scent of middle note compounds is usually more mellow and "rounded". Scents from this note class disappear anywhere from twenty minutes to one hour after the application of a perfume. Lavender and rose scents are
15 typical middle notes.

Base notes are the scent of a perfume that appears close to the departure of the middle notes. The base and middle notes together are the main theme of a perfume. Base notes bring depth and solidity to a perfume. Compounds of this
20 class are often the fixatives used to hold and boost the strength of the lighter top and middle notes. Consisting of large, heavy molecules that evaporate slowly, compounds of this class of scents are typically rich and "deep" and are usually not perceived until 30 minutes after the application of the perfume or during the period of perfume dry-down. Some base notes can still be detectable
25 in excess of twenty-four hours after application, particularly the animalic and musk notes.

The present disclosure provides a composition, comprising:

- a) a compound of Formula (I) or a salt, solvate or stereoisomer thereof:



wherein

R_1 , R_2 , R_3 and R_4 are independently selected from H, oxo, optionally substituted alkyl, optionally substituted alkenyl; and

- 5 R_5 , R_6 , R_7 , R_8 and R_9 are independently selected from H, oxo, optionally substituted alkyl, optionally substituted alkenyl;

wherein the compound of Formula (I) is characterised by a concentration of at least 80 ppm relative to the composition.

- 10 The composition refers to a distribution of the individual substances that constitute the entity, i.e. components will make up a composition. The composition may be a perfume composition. The perfume composition may be used in soaps, detergents, cosmetics, toiletries, fine fragrances, household products, aromatherapy and pesticides. The composition may be used as a top
- 15 note, middle note and/or base note. The composition may be a food product, or a packaging suitable for containing food.

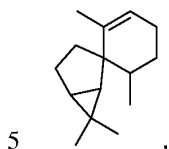
In some embodiments, R_1 , R_2 , R_3 and R_4 are independently optionally substituted alkyl. In some embodiments, R_1 , R_2 , R_3 and R_4 are independently

20 optionally substituted C_1 - C_4 alkyl. The alkyl may be methyl, ethyl, propyl iso-propyl, n-butyl, t-butyl, sec-butyl or iso-butyl. The optional substituent may be halo, oxo, alkoxy, or amino.

- In some embodiments, R_5 , R_6 , R_7 , R_8 and R_9 are independently selected from H,
- 25 or optionally substituted alkyl. In some embodiments, R_5 , R_6 , R_7 , R_8 and R_9 are independently selected from H, or optionally substituted C_1 - C_4 alkyl. In some embodiments, R_5 , R_6 , R_7 , R_8 and R_9 are independently selected from optionally substituted C_1 - C_4 alkyl. The alkyl may be methyl, ethyl, propyl iso-propyl, n-butyl, t-butyl, sec-butyl or iso-butyl. The optional substituent may be halo, oxo,

alkoxy, or amino. In some embodiments, R₅, R₆, R₇, R₈ and R₉ are independently H.

In some embodiments, the compound of Formula (I) is

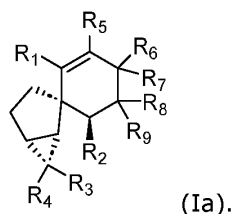


"Isomer" includes especially optical isomers or stereoisomers (for example essentially pure enantiomers, essentially pure diastereomers, and mixtures thereof) as well as conformation isomers (i.e. isomers that differ only in their
10 angles of at least one chemical bond), position isomers (particularly tautomers), and geometric isomers (e.g. cis-trans isomers).

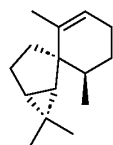
Compounds described herein can comprise one or more asymmetric centers, and thus can exist in various isomeric forms, e.g., enantiomers and/or
15 diastereomers. For example, the compounds described herein can be in the form of an individual enantiomer, diastereomer or geometric isomer, or can be in the form of a mixture of stereoisomers, including racemic mixtures and mixtures enriched in one or more stereoisomer. Isomers can be isolated from mixtures by methods known to those skilled in the art, including chiral high pressure
20 liquid chromatography (HPLC) and the formation and crystallization of chiral salts; or preferred isomers can be prepared by asymmetric syntheses. The invention additionally encompasses compounds described herein as individual isomers substantially free of other isomers, and alternatively, as mixtures of various isomers. "Optically-enriched," as used herein, means that the compound
25 is made up of a significantly greater proportion of one enantiomer. In certain embodiments the compound of the present invention is made up of at least about 90% by weight of a preferred enantiomer. In other embodiments the compound is made up of at least about 95%, 98%, or 99% by weight of a preferred enantiomer. Preferred enantiomers may be isolated from racemic
30 mixtures by any method known to those skilled in the art, including chiral high

pressure liquid chromatography (HPLC) and the formation and crystallization of chiral salts or prepared by asymmetric syntheses. See, for example, Jacques et al., *Enantiomers, Racemates and Resolutions* (Wiley Interscience, New York, 1981); Wilen et al., *Tetrahedron* 33:2725 (1977); Eliel, *Stereochemistry of Carbon Compounds* (McGraw-Hill, NY, 1962); and Wilen, *Tables of Resolving Agents and Optical Resolutions* p. 268 (E.L. Eliel, Ed., Univ. of Notre Dame Press, Notre Dame, IN 1972).

In some embodiments, the compound of Formula (I) is a compound of Formula (Ia):



In some embodiments, the compound of Formula (I) is



. This compound is labelled as Compound 1 herein.

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The compound of the invention can be salt thereof. Suitable salts include, but are not limited to salts of inorganic acids such as hydrochloric, sulphuric, phosphoric, nitric, carbonic, boric, sulfamic, and hydrobromic acids, or salts of pharmaceutically acceptable organic acids such as acetic, propionic, butyric, tartaric, maleic, hydroxymaleic, fumaric, maleic, citric, lactic, mucic, gluconic, benzoic, succinic, oxalic, phenylacetic, methanesulphonic, toluenesulphonic, benzenesulphonic, salicylic sulphonic, aspartic, glutamic, edetic, stearic, palmitic, oleic, lauric, pantothenic, tannic, ascorbic and valeric acids.

25 Base salts include, but are not limited to, those formed with pharmaceutically acceptable cations, such as sodium, potassium, lithium, calcium, magnesium,

ammonium and alkylammonium. In particular, the present invention includes within its scope cationic salts eg sodium or potassium salts, or alkyl esters (eg methyl, ethyl) of the phosphate group.

- 5 Basic nitrogen-containing groups may be quarternised with such agents as lower alkyl halide, such as methyl, ethyl, propyl, and butyl chlorides, bromides and iodides; dialkyl sulfates like dimethyl and diethyl sulfate; and others.

The compound of the invention may be in crystalline form either as the free
10 compound or as a solvate (e.g. hydrate) and it is intended that both forms are within the scope of the present invention. Methods of solvation are generally known within the art.

The intensity of the odour may be determined via a threshold value
15 determination. A threshold value of an odour is the concentration of a substance in the relevant gas space at which an odour impression may just still be perceived by a representative test panel, although it no longer has to be defined.

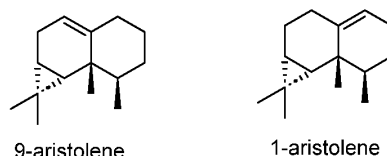
In some embodiments, the compound of Formula (I) is characterised by a
20 concentration of at least 100 ppm relative to the composition.

In some embodiments, the compound of Formula (I) is characterised by a concentration of about 0.01 wt% to about 30 wt% relative to the composition. In other embodiments, the concentration is about 0.01 wt% to about 25 wt%,
25 about 0.01 wt% to about 20 wt%, about 0.01 wt% to about 18 wt%, about 0.01 wt% to about 16 wt%, about 0.01 wt% to about 14 wt%, about 0.01 wt% to about 12 wt%, about 0.01 wt% to about 10 wt%, about 0.01 wt% to about 8 wt%, about 0.01 wt% to about 6 wt%, about 0.01 wt% to about 4 wt%, or about 0.01 wt% to about 2 wt%.

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In some embodiments, the compound of Formula (I) is characterised by a woody and/or earthy scent.

As synthesised, a sample comprising compound 1 may further comprise impurities or by-products, which may be volatile compounds. For example, 9-aristolene and/or 1-aristolene may be present. Depending on the degree of purification, these impurities may also be added to the composition and may
5 play a role in providing the scent profile.



In some embodiments, the composition further comprises 9-aristolene. In some
10 embodiments, the 9-aristolene is characterised by a concentration of at least 20 ppm relative to the composition. In other embodiments, the concentration is at least 30 ppm or at least 50 ppm.

In some embodiments, 9-aristolene is characterised by a concentration of about
15 0.01 wt% to about 10 wt% relative to the composition. In other embodiments, the concentration is about 0.01 wt% to about 9 wt%, about 0.01 wt% to about 8 wt%, about 0.01 wt% to about 7 wt%, about 0.01 wt% to about 6 wt%, about 0.01 wt% to about 5 wt%, about 0.01 wt% to about 4 wt%, about 0.01 wt% to about 3 wt%, about 0.01 wt% to about 2 wt%, about 0.01 wt% to about 1 wt%,
20 about 0.01 wt% to about 0.9 wt%, about 0.01 wt% to about 0.8 wt%, about 0.01 wt% to about 0.7 wt%, about 0.01 wt% to about 0.6 wt%, about 0.01 wt% to about 0.5 wt%, about 0.01 wt% to about 0.4 wt%, about 0.01 wt% to about 0.3 wt%, about 0.01 wt% to about 0.2 wt%, or about 0.01 wt% to about 0.1 wt%.

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The presence of the by-products may alter the sensory profile of compound of Formula (I). In some embodiments, the composition is characterised by a woody, earthy and medicinal scent. This scent may be due to a combinatory effect of compound of Formula (I) and 9-aristolene.

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In some embodiments, the composition further comprises 1-aristolene. In some embodiments, the 1-aristolene is characterised by a concentration of less than 20 ppm relative to the composition. In other embodiments, the concentration is less than 15 ppm, or less than 10 ppm. 1-aristolene does not provide an odour.

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In some embodiments, 1-aristolene is characterised by a concentration of about 0.01 wt% to about 10 wt% relative to the composition. In other embodiments, the concentration is about 0.01 wt% to about 9 wt%, about 0.01 wt% to about 8 wt%, about 0.01 wt% to about 7 wt%, about 0.01 wt% to about 6 wt%, about 0.01 wt% to about 5 wt%, about 0.01 wt% to about 4 wt%, about 0.01 wt% to about 3 wt%, about 0.01 wt% to about 2 wt%, about 0.01 wt% to about 1 wt%, about 0.01 wt% to about 0.9 wt%, about 0.01 wt% to about 0.8 wt%, about 0.01 wt% to about 0.7 wt%, about 0.01 wt% to about 0.6 wt%, about 0.01 wt% to about 0.5 wt%, about 0.01 wt% to about 0.4 wt%, about 0.01 wt% to about 0.3 wt%, about 0.01 wt% to about 0.2 wt%, or about 0.01 wt% to about 0.1 wt%.

In some embodiments, the composition is characterised by a ratio of the compound of Formula (I) to the impurity (9-aristolene and 1-aristolene) of about 2:1 to about 6:1. In other embodiments, the ratio is about 2:1 to about 4:1.

In some embodiments, the method is characterised by a ratio of the compound of Formula (I) to 9-aristolene of about 2:1 to about 6:1. In other embodiments, the ratio is about 2:1 to about 4:1.

In some embodiments, the compound of Formula (I) is a component in a top note. In some embodiments, the compound of Formula (I) is a component in a middle note. In some embodiments, the compound of Formula (I) is a component in a base note.

In some embodiments, the composition further comprises another aroma chemical. The aroma chemical may be selected from, but not limited to, geranyl

acetate, alpha-hexylcinnamaldehyde, 2-phenoxyethyl isobutyrate, dihydromyrcenol, methyl dihydrojasmonate, 4,6,6,7,8,8-hexamethyl-1,3,4,6,7,8-hexahydrocyclopenta[g]benzopyran, tetrahydrolinalool, ethyllinalool, benzyl salicylate, 2-methyl-3-(4-tert-butylphenyl)propanal, 5 cinnamyl alcohol, 4,7-methano-3a,4,5,6,7,7a-hexahydro-5-indenyl acetate and/or 4,7-methano-3a,4,5,6,7,7a-hexahydro-6-indenyl acetate, citronellol, citronellyl acetate, tetrahydrogeraniol, vanillin, linalyl acetate, styrolyl acetate, octahydro-2,3,8,8-tetramethyl-2-acetonaphthone and/or 2-acetyl-1,2,3,4,6,7,8-octahydro-2,3,8,8-tetramethylnaphthalene, hexyl salicylate, 4-10 tert-butylcyclohexyl acetate, 2-tertbutylcyclohexyl acetate, alpha-ionone, n-alpha-methylionone, alpha-isomethylionone, coumarin, terpinyl acetate, 2-phenylethyl alcohol, 4-(4-hydroxy-4-methylpentyl)-3-cyclohexene-carboxaldehyde, alpha-amylcinnamaldehyde, ethylene brassylate, (E)- and/or (Z)-3-methylcyclopentadec-5-enone, 15-pentadec-11-enolide and/or 15-15 pentadec-12-enolide, 15-cyclo-pentadecanolide, 1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthalenyl)ethanone, 2-isobutyl-4-methyltetrahydro-2H-pyran-4-ol, 2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol, cis-3-hexenyl acetate, trans-3-hexenyl acetate, trans-2/cis-6-nonadienol, 2,4-dimethyl-3-cyclohexenecarboxaldehyde, 2,4,4,7-tetramethyloct-6-en-3-one, 2,6-dimethyl-5-hepten-1-al, borneol, 3-(3-isopropylphenyl)butanal, 2-methyl-3-(3,4-methylenedioxyphenyl)propanal, 3-(4-ethylphenyl)-2,2-dimethylpropanal, 7-methyl-2H-1,5-benzodioxepin-3(4H)-one, 3,3,5-trimethylcyclohexylacetate, 2,5,5-trimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalen-2-ol, 3-(4-tert-butylphenyl)-propanal, ethyl 2-25 methylpentanoate, ethoxymethoxycyclododecane, 2,4-dimethyl-4,4a,5,9b-tetrahydroindeno[1,2-d][1,3]dioxine, (2-tert-butylcyclohexyl)acetate and 3-[5,5,6-trimethylbicyclo[2.2.1]hept-2-yl]cyclohexan-1-ol.

Further aroma chemicals may be selected from S. Arctander, Perfume and 30 Flavor Chemicals, Vol. I and II, Montclair, N. J., 1969, or K. Bauer, D. Garbe and H. Surburg, Common Fragrance and Flavor Materials, 4th Ed., Wiley- VCH, Weinheim 2001. For example, aroma chemicals may be:

- i) extracts from natural raw materials such as essential oils, concretes, absolutes, resins, resinoids, balsams, tinctures such as e.g. ambergris tincture; amyris oil; angelica seed oil; angelica root oil; aniseed oil; valerian oil; basil oil; tree moss absolute; bay oil; mugwort oil; benzoin resin; bergamot oil; beeswax absolute; birch tar oil; bitter almond oil; savory oil; buchu leaf oil; cabreuva oil; cade oil; calmus oil; camphor oil; cananga oil; cardamom oil; cascarilla oil; cassia oil; cassia absolute; castoreum absolute; cedar leaf oil; cedar wood oil; cistus oil; citronella oil; lemon oil; copaiba balsam; copaiba balsam oil; coriander oil; costus root oil; cumin oil; cypress oil; davana oil; dill weed oil; dill seed oil; Eau de brouts absolute; oak moss absolute; elemi oil; tarragon oil; eucalyptus citriodora oil; eucalyptus oil; fennel oil; pine needle oil; galbanum oil; galbanum resin; geranium oil; grapefruit oil; guaiacwood oil; gurjun balsam; gurjun balsam oil; helichrysum absolute; helichrysum oil; ginger oil; iris root absolute; iris root oil; jasmine absolute; calmus oil; camomile oil blue; roman camomile oil; carrot seed oil; cascarilla oil; pine needle oil; spearmint oil; caraway oil; labdanum oil; labdanum absolute; labdanum resin; lavandin absolute; lavandin oil; lavender absolute; lavender oil; lemongrass oil; lovage oil; lime oil distilled; lime oil pressed; linalool oil; litsea cubeba oil; laurel leaf oil; mace oil; marjoram oil; mandarin oil; massoia bark oil; mimosa absolute; musk seed oil; musk tincture; clary sage oil; nutmeg oil; myrrh absolute; myrrh oil; myrtle oil; clove leaf oil; clove flower oil; neroli oil; olibanum absolute; olibanum oil; opopanaxoil; orange blossom absolute; orange oil; origanum oil; palmarosa oil; patchouli oil; perilla oil; peru balsam oil; parsley leaf oil; parsley seed oil; petitgrain oil; peppermint oil; pepper oil; pimento oil; pine oil; pennyroyal oil; rose absolute; rose wood oil; rose oil; rosemary oil; Dalmatian sage oil; Spanish sage oil; sandalwood oil; celery seed oil; spike-lavender oil; star anise oil; styrax oil; tagetes oil; fir needle oil; tea tree oil; turpentine oil; thyme oil; tolubalsam; tonka absolute; tuberose absolute; vanilla extract; violet leaf absolute; verbena oil; vetiver oil; juniper berry oil; wine lees oil; wormwood oil; winter green oil; hyssop oil; civet absolute; cinnamon leaf oil; cinnamon bark oil, and fractions thereof, or ingredients isolated therefrom;
- ii) individual fragrances from the group of hydrocarbons, such as e.g. 3 carene;

- alpha-pinene; beta-pinene; alphaterpinene; gamma-terpinene; p-cymene; bisabolene; camphene; caryophyllene; cedrene; farnesene; limonene; longifolene; myrcene; ocimene; valencene; (E,Z)-1,3,5-undecatriene; styrene; diphenylmethane; the aliphatic alcohols such as e.g. hexanol; octanol; 3-octanol; 2,6-dimethylheptanol; 2-methyl-2-heptanol; 2-methyl-2-octanol; (E)-2-hexenol; (E)- and (Z)-3-hexenol; 1-octen-3-ol; mixture of 3,4,5,6,6-pentamethyl-3/4-hepten-2-ol and 3,5,6,6-tetramethyl-4-methyleneheptan-2-ol; (E,Z)-2,6-nonadienol; 3,7-dimethyl-7-methoxyoctan-2-ol; 9-decenol; 10-undecenol; 4-methyl-3-decen-5-ol;
- 10 iii) the aliphatic aldehydes and acetals thereof such as e.g. hexanal; heptanal; octanal; nonanal; decanal; undecanal; dodecanal; tridecanal; 2-methyloctanal; 2-methylnonanal; (E)-2-hexenal; (Z)-4-heptenal; 2,6-dimethyl-5-heptenal; 10-undecenal; (E)-4-decenal; 2-dodecenal; 2,6,10-trimethyl-9-undecenal;
- 15 2,6,10-trimethyl-5,9-undecadienal; heptanal diethyl acetal; 1,1-dimethoxy-2,2,5-trimethyl-4-hexene; citronellyloxyacetaldehyde; (E/Z)-1-(1-methoxypropoxy)-hex-3-ene; the aliphatic ketones and oximes thereof such as e.g. 2-heptanone; 2-octanone; 3-octanone; 2-nonanone; 5-methyl-3-heptanone; 5-methyl-3-heptanone oxime; 2,4,4,7-tetramethyl-6-octen-3-one;
- 20 6-methyl-5-hepten-2-one;
- iv) the aliphatic sulfur-containing compounds such as e.g. 3-methylthiohexanol; 3-methylthiohexyl acetate; 3-mercaptohexanol; 3-mercaptohexyl acetate; 3-mercaptohexyl butyrate; 3-acetylthiohexyl acetate; 1-menthene-8-thiol;
- 25 v) the aliphatic nitriles such as e.g. 2-nonenenitrile; 2-undecenitrile; 2-tridecenitrile; 3,12-tridecadienenitrile; 3,7-dimethyl-2,6-octadienenitrile; 3,7-dimethyl-6-octenenitrile;
- 30 vi) the esters of aliphatic carboxylic acids such as e.g. (E) and (Z)-3-hexenyl formate; ethyl acetoacetate; isoamyl acetate; hexyl acetate; 3,5,5-trimethylhexyl acetate; 3-methyl-2-butenyl acetate; (E)-2-hexenyl acetate; (E) and (Z)-3-hexenyl acetate; octyl acetate; 3-octyl acetate; 1-octen-3-yl

acetate; ethyl butyrate; butyl butyrate; isoamyl butyrate; hexyl butyrate; (E) and (Z)-3-hexenyl isobutyrate; hexyl crotonate; ethyl isovalerate; ethyl 2-methylpentanoate; ethylhexanoate; allyl hexanoate; ethyl heptanoate; allyl heptanoate; ethyl octanoate; ethyl (E,Z)-2,4-decadienoate; methyl 2-octinate;
5 methyl 2-noninate; allyl 2-isoamylacetate; methyl-3,7-dimethyl-2,6-octadienoate; 4-methyl-2-pentylcrotonate;

vii) the acyclic terpene alcohols such as e.g. geraniol; nerol; linalool; lavandulol; nerolidol; farnesol; tetrahydrolinalool; 2,6-dimethyl-7-octen-2-ol; 2,6-
10 dimethyloctan-2-ol; 2-methyl-6-methylene-7-octen-2-ol; 2,6-dimethyl-5,7-octadien-2-ol; 2,6-dimethyl-3,5-octadien-2-ol; 3,7-dimethyl-4,6-octadien-3-ol; 3,7-dimethyl-1,5,7-octatrien-3-ol; 2,6-dimethyl-2,5,7-octatrien-1-ol; and the formates, acetates, propionates, isobutyrate, butyrate, isovalerate, pentanoates, hexanoates, crotonates, tiglinates and 3-methyl-2-butenes
15 thereof;

ix) the acyclic terpene aldehydes and ketones such as e.g. geranial; neral; citronellal; 7-hydroxy-3,7-dimethyloctanal; 7-methoxy-3,7-dimethyloctanal; 2,6,10-trimethyl-9-undecenal; geranyl acetone; as well as the dimethyl and
20 diethyl-acetals of geranial, neral, 7-hydroxy-3,7-dimethyloctanal;

ix) the cyclic terpene alcohols such as e.g. menthol; isopulegol; alpha-terpineol; terpineol-4-ol; menthan-8-ol; menthan-1-ol; menthan-7-ol; borneol; isoborneol; linalool oxide; nopol; cedrol; ambrinol; vetiverol; guajol; and the formates,
25 acetates, propionates, isobutyrate, butyrate, isovalerate, pentanoates, hexanoates, crotonates, tiglinates and 3-methyl-2-butenes thereof;

x) the cyclic terpene aldehydes and ketones such as e.g. menthone; isomenthone; 8-mercaptomenthan-3-one; carvone; camphor; fenchone; alpha-ionone; beta-ionone; alpha-n-methylionone; beta-n-methylionone; alpha-isomethylionone; beta-isomethylionone; alpha-irone; alpha-damascone; beta-damascone; beta-damascenone; delta-damascone; gamma-damascone; 1-(2,4,4-trimethyl-2-cyclohexen-1-yl)-2-buten-1-one; 1,3,4,6,7,8a-hexahydro-

1,1,5,5-tetramethyl-2H-2,4a-methano_,naphthalene-8(5H)-one; 2-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2-butenal; nootkatone; dihydronootkatone; 4,6,8-megastigmatrien-3-one; alpha-sinensal; beta-sinensal; acetylated cedar wood oil (methyl cedryl ketone);

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xi) the cyclic alcohols such as e.g. 4-tert-butylcyclohexanol; 3,3,5-trimethylcyclohexanol; 3-isocamphylcyclohexanol; 2,6,9-trimethyl-Z2, Z5,E9-cyclododecatrien-1-ol; 2-isobutyl-4-methyltetrahydro-2H-pyran-4-ol;

10 xii) the cycloaliphatic alcohols such as e.g. alpha-3,3-
trimethylcyclohexylmethanol; 1 (4-isopropylcyclohexyl)ethanol; 2-methyl-4-
(2,2,3-trimethyl-3-cyclopent-1-yl)butanol; 2-methyl-4-(2,2,3 trimethyl-3-cycl
opent-1-yl) -2-buten-1-ol; 2-ethyl-4-(2,2,3-trimethyl-3 cyclopent-1-yl)-2-
buten-1-ol; 3-methyl-5-(2,2,3 trimethyl-3-cyclopent-1-yl)pentan-2 ol; 3-
15 methyl-5-(2,2,3-trimethyl-3-cyclopent-1-yl)-4-penten-2-ol; 3,3-dimethyl-5-
(2,2,3-trimethyl-3-cyclopent-1-yl)-4-penten-2-ol; 1-(2,2,6-
trimethylcyclohexyl)pentan-3-ol; 1-(2,2,6-trimethylcyclohexyl)hexan-3-ol;

xiii) the cyclic and cycloaliphatic ethers such as e.g. cineol; cedryl methyl ether;
20 cyclododecyl methyl ether; 1,1-dimethoxycyclododecane;
(ethoxymethoxy)cyclo-dodecane; alpha-cedrene epoxide; 3a,6,6,9a-
tetramethyldodecahydronaphtho[2,1-b]furan; 3a-ethyl-6,6,9a-
trimethyldodecahydro-naphtho[2,1-b]furan; 1,5,9-trimethyl-13-oxabicyclo-
[10.1.0]trideca-4,8-diene; rose oxide; 2-(2,4-dimethyl-3-cyclohexen-1-yl)-5-
25 methyl-5-(1-methylpropyl)-1,3-dioxane;

xiv) the cyclic and macrocyclic ketones such as e.g. 4-tert-butylcyclohexanone; 2,2,5 trimethyl-5-pentylcyclopentanone; m 2-heptylcyclopentanone; 2-pentylcyclo-pentanone; 2-hydroxy-3-methyl-2-cyclopenten-1-one; 3-methyl-30 cis-2-penten-1-yl-2 cyclopenten-1-one; 3-methyl-2-pentyl-2-cyclopenten-1-one; 3-methyl-4-cyclopenta-decenone; 3-methyl-5-cyclopentadecenone; 3-methylcyclopentadecanone; 4-(1-ethoxyvinyl)-3,3,5,5-tetramethylcyclohexanone; 4-tertpentylcyclohexanone; 5-cyclohexadecen-1-

one; 6,7-dihydro-1,1,2,3,3-pentamethyl-4(5H)-indanone; 8-cyclo-hexadecen-1-one; 7-cyclohexadecen-1-one; (7/8)-cyclohexadecen-1-one; 9 cyclo-heptadecen-1-one; cyclopentadecanone; cyclohexadecanone;

5 xv) the cycloaliphatic aldehydes such as e.g. 2,4-dimethyl-3-cyclohexenecarbaldehyde; 2 methyl-4-(2,2,6-trimethylcyclohexen-1-yl)-2-butenal; 4-(4-hydroxy-4-methylpentyl)-3 cyclohexene carbaldehyde; 4-(4-methyl-3-penten-1-yl)-3-cyclohexenecarbaldehyde;

10 xvi) the cycloaliphatic ketones such as e.g. 1-(3,3-dimethylcyclohexyl)-4-penten-1-one; 2,2 dimethyl-1-(2,4-dimethyl-3-cyclohexen-1-yl)-1-propanone; 1-(5,5-dimethyl-1 cyclohexen-1-yl)-4-penten-1-one; 2,3,8,8-tetramethyl-1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl methyl ketone; methyl 2,6,10-trimethyl-2,5,9-cyclododecatrienyl ketone; tert-butyl (2,4-dimethyl-3-
15 cyclohexen-1-yl) ketone;

xvii) the esters of cyclic alcohols such as e.g. 2-tert-butylcyclohexyl acetate; 4-tert-butylcyclohexyl acetate; 2-tert-pentylcyclohexylacetate; 4-tert-pentylcyclohexyl acetate; 3,3,5-trimethylcyclohexyl acetate; decahydro-2-
20 naphthyl acetate; 2-cyclopentylcyclopentyl crotonate; 3-pentyltetrahydro-2H-pyran-4-yl acetate; decahydro-2,5,5,8a-tetramethyl-2-naphthyl acetate; 4,7-methano-3a,4,5,6,7,7a-hexahydro-5 or 6-indenyl acetate; 4,7-methano-3a,4,5,6,7,7a-hexahydro-5 or 6 indenyl propionate; 4,7-methano-3a,4,5,6,7,7a-hexahydro-5 or 6-indenyl isobutyrate; 4,7 methano-octahydro-5
25 or 6-indenyl acetate;

xiix) the esters of cycloaliphatic alcohols such as e.g. 1-cyclohexylethyl crotonate;

30 xix) the esters of cycloaliphatic carboxylic acids such as e.g. allyl 3-cyclohexylpropionate; allyl cyclohexyloxyacetate; cis and trans-methyl dihydrojasmonate; cis and trans-methyl jasmonate; methyl 2-hexyl-3-oxocyclopentanecarboxylate; ethyl 2-ethyl-6,6 dimethyl-2-

cyclohexenecarboxylate; ethyl 2,3,6,6-tetramethyl-2 cyclohexene-carboxylate;
ethyl 2-methyl-1,3-dioxolane-2-acetate;

xx) the araliphatic alcohols such as e.g. benzyl alcohol; 1-phenylethyl alcohol,
5 2 phenylethyl alcohol, 3-phenylpropanol; 2- phenyl propanol; 2-
phenoxyethanol; 2,2-dimethyl-3-phenylpropanol; 2,2-dimethyl-3-(3-
methylphenyl)propanol; 1,1-dimethyl-2 phenylethyl alcohol; 1,1-dimethyl-3-
phenylpropanol; 1-ethyl-1-methyl-3-phenylpropanol; 2-methyl-5-
phenylpentanol; 3-methyl-5-phenylpentanol; 3-phenyl-2-propen-1-ol; 4-
10 methoxy-, benzyl alcohol; 1-(4-isopropylphenyl)ethanol;

xxi) the esters of araliphatic alcohols and aliphatic carboxylic acids such as e.g.
benzyl acetate; benzyl propionate; benzyl isobutyrate; benzyl isovalerate; 2-
phenylethyl acetate; 2-phenylethyl propionate; 2-phenylethyl isobutyrate; 2
15 phenylethyl isovalerate; 1 phenylethyl acetate; alpha-trichloromethylbenzyl
acetate; alpha,alpha-dimethylphenylethylacetate; alpha,alpha-
dimethylphenylethyl butyrate; cinnamyl acetate; 2-phenoxyethyl isobutyrate;
4-methoxybenzylacetate;

20 the araliphatic ethers such as e.g. 2-phenylethyl methyl ether; 2 phenylethyl
isoamyl ether; 2-phenylethyl 1-ethoxyethyl ether; phenylacetaldehyde dimethyl
acetal; phenylacetaldehyde diethyl acetal; hydratropaaldehyde dimethylacetal;
phenylacetaldehyde glycerol acetal; 2,4,6-trimethyl-4-phenyl-1,3-dioxane;
4,4a,5,9b-tetrahydroindeno[1,2-d]-m-dioxine; 4,4a,5,9b-tetrahydro-2,4-
25 dimethylindeno[1,2-d]-m dioxine;

xxii) the aromatic and araliphatic aldehydes such as e.g. benzaldehyde;
phenylacetaldehyde; 3-phenylpropanal; hydratropaaldehyde; 4-
methylbenzaldehyde; 4 methylphenylacetaldehyde; 3-(4-ethylphenyl)-2,2-
30 dimethylpropanal; 2-methyl-3-(4-isopropylphenyl)propanal; 2-methyl-3-(4-
tert-butylphenyl)propanal; 2-methyl-3-(4-isobutylphenyl)propanal; 3-(4-tert-
butylphenyl)propanal; cinnamaldehyde; alpha-butylcinnamaldehyde; alpha-
amylcinnamaldehyde; alpha-hexylcinnamaldehyde; 3 methyl-5-

phenylpentanal; 4-methoxybenzaldehyde; 4-hydroxy-3-methoxybenzaldehyde; 4-hydroxy-3-ethoxybenzaldehyde; 3,4-methylenedioxybenzaldehyde; 3,4-dimethoxybenzaldehyde; 2-methyl-3-(4-methoxyphenyl)propanal; 2-methyl-3-(4-methylenedioxyphenyl)propanal;

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xxiii) the aromatic and aliphatic ketones such as e.g. acetophenone; 4-methylacetophenone; 4-methoxyacetophenone; 4-tert-butyl-2,6-dimethylacetophenone; 4-phenyl-2-butanone; 4-(4-hydroxyphenyl)-2-butanone; 1-(2-naphthalenyl)-ethanone; 2-benzofuranylethanone; (3-methyl-2-benzofuranyl)ethanone; benzophenone; 1,1,2,3,3,6-hexamethyl-5-indanyl methyl ketone; 6-tert-butyl-1,1-dimethyl-4-indanyl methyl ketone; 1-[2,3-dihydro-1,1,2,6-tetramethyl-3-(1-methylethyl)-1H-5-indenyl]ethanone; 5',6',7',8'-tetrahydro-3',5',5',6',8',8'-hexamethyl-2-acetonaphthone;

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xxiv) the aromatic and aliphatic carboxylic acids and esters thereof such as e.g. benzoic acid; phenylacetic acid; methylbenzoate; ethyl benzoate; hexyl benzoate; benzyl benzoate; methyl phenylacetate; ethyl phenylacetate; geranyl phenylacetate; phenylethyl phenylacetate; methyl cinnamate; ethyl cinnamate; benzyl cinnamate; phenylethyl cinnamate; cinnamyl cinnamate; allyl phenoxyacetate; methyl salicylate; isoamyl salicylate; hexyl salicylate; cyclohexylsalicylate; cis-3-hexenyl salicylate; benzyl salicylate; phenylethyl salicylate; methyl 2,4-dihydroxy-3,6-dimethylbenzoate; ethyl 3-phenylglycidate; ethyl 3-methyl-3-phenylglycidate;

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xxv) the nitrogen-containing aromatic compounds such as e.g. 2,4,6-trinitro-1,3-dimethyl-5-tert-butylbenzene; 3,5-dinitro-2,6-dimethyl-4-tert-butylacetophenone; cinnamionitrile; 3-methyl-5-phenyl-2-pentenitrile; 3-methyl-5-phenylpentanonitrile; methyl anthranilate; methyl-N-methylanthranilate; Schiffbases of methyl anthranilate with 7-hydroxy-3,7-dimethyloctanal, 2-methyl-3-(4-tert-butylphenyl)propanal or 2,4-dimethyl-3-cyclohexenecarbaldehyde; 6-isopropylquinoline; 6-isobutylquinoline; 6-sec-butylquinoline; 2-(3-phenylpropyl)pyridine; indole; skatole; 2-methoxy-3-isopropylpyrazine; 2-isobutyl-3-methoxypyrazine;

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xxvi) the phenols, phenyl ethers and phenyl esters such as e.g. estragole; anethole; eugenol; eugenyl methyl ether; isoeugenol; isoeugenyl methyl ether; thymol; carvacrol; diphenyl ether; beta-naphthyl methyl ether; beta-naphthylethyl ether; beta-naphthyl isobutyl ether; 1,4-dimethoxybenzene; eugenyl acetate; 2-methoxy-4-methylphenol; 2-ethoxy-5-(1-propenyl)phenol; p-cresyl phenylacetate;

xxvii) the heterocyclic compounds such as e.g. 2,5-dimethyl-4-hydroxy-2H-furan-3-one; 2 ethyl-4-hydroxy-5-methyl-2Hfuran-3-one; 3-hydroxy-2-methyl-4H-pyran-4-one; 2 ethyl-3-hydroxy-4H-pyran-4-one;

xxiix) the lactones such as e.g. 1,4-octanolide; 3-methyl-1,4-octanolide; 1,4-nonanolide; 1,4-decanolide; 8-decen-1,4-olide; 1,4-undecanolide; 1,4-dodecanolide; 1,5-decanolide; 1,5-dodecanolide; 4-methyl-1,4-decanolide; 1,15-pentadecanolide; cis and trans-11-pentadecen-1,15-olide; cis and trans-12-pentadecen-1,15-olide; 1,16-hexadecanolide; 9-hexadecen-1,16-olide; 10-oxa-1,16-hexadecanol ide; 11 -oxa-1,16-hexadecanol ide; 12-oxa-1,16-hexadecanolide; ethylene 1,12-dodecanedioate; ethylene 1,13-tridecanedioate; coumarin; 2,3-dihydrocoumarin; octahydrocoumarin.

In some embodiments, the composition further comprises at least one carrier and/or auxiliary agent. "Carrier" means a material or component which is practically neutral from a odourant point of view, i.e. a material that does not significantly alter the organoleptic properties of odourants. The term "auxiliary agent" refers to ingredients that might be employed in a perfume composition for reasons not specifically related to the olfactive performance of said composition. For example, an auxiliary agent may be an ingredient that acts as an aid to processing a fragrance ingredient or ingredients, or a composition containing said ingredient(s), or it may improve handling or storage of a fragrance ingredient or composition containing same. It might also be an ingredient that provides additional benefits such as imparting color or texture. It might also be an ingredient that imparts light resistance or chemical stability

to one or more ingredients contained in a perfume composition. The carrier and/or auxiliary agent may be a surfactant, oil component, antioxidant, deodorant-active agents and/or solvent.

- 5 The solvent used in perfume may affect how the fragrance smells. For example, benzyl acetate has a flowery smell and is often used in floral fragrances. Phenethyl alcohol gives off a delicate honey-like scent and is found naturally in many foods such as apricots, coffee beans, and honey. It's also used for its spicy cinnamon fragrance. Cinnamaldehyde imparts the typical flavor of cinnamon
10 with an odor similar to the oil of cloves, while tetrahydro furfuryl ethyl ether can give off the scent of chocolate. Volatile alcohols such as methanol, ethanol and propanol may also be used. Other solvents include, methylene chloride, limonene, linalool, synthetic musks, phthalates, turpentine, pinene, myrcene, terpinolene, dihydro terpineol, and terpineol.

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In some embodiments, the solvent is selected from the group consisting of ethanol, isopropanol, diethylene glycol monoethyl ether, glycerol, propylene glycol, 1,2-butylene glycol, dipropylene glycol, triethyl citrate, isopropyl myristate or a mixture thereof.

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In some embodiments, the solvent is characterised by a concentration of about 30 wt% to about 99 wt% relative to the composition. In other embodiments, the concentration is about 40 wt% to about 99 wt%, about 50 wt% to about 99 wt%, about 60 wt% to about 99 wt%, or about 70 wt% to about 99 wt%.

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- In some embodiments, the oil component is selected from, but not limited to, Guerbet alcohols based on fatty alcohols containing 6 to 18, preferably 8 to 10, carbon atoms and other additional esters, such as myristyl myristate, myristyl palmitate, myristyl stearate, myristyl isostearate, myristyl oleate, myristyl
30 behenate, myristyl erucate, cetyl myristate, cetyl palmitate, cetyl stearate, cetyl isostearate, cetyl oleate, cetyl behenate, cetyl erucate, stearyl myristate, stearyl palmitate, stearyl stearate, stearyl isostearate, stearyl oleate, stearyl behenate, stearyl erucate, isostearyl myristate, isostearyl palmitate, isostearyl

stearate, isostearyl isostearate, isostearyl oleate, isostearyl behenate, isostearyl oleate, oleyl myristate, oleyl palmitate, oleyl stearate, oleyl isostearate, oleyl oleate, oleyl behenate, oleyl erucate, behenyl myristate, behenyl palmitate, behenyl stearate, behenyl isostearate, behenyl oleate, behenyl behenate, behenyl erucate, erucyl myristate, erucyl palmitate, erucyl stearate, erucyl isostearate, erucyl oleate, erucyl behenate and erucyl erucate. Also suitable are esters of C18-C38 alkyl-hydroxycarboxylic acids with linear or branched C6-C22 fatty alcohols, such as dioctyl malate, esters of linear and/or branched fatty acids with polyhydric alcohols (for example propylene glycol, dimer dial or trimer triol), triglycerides based on C6-C10 fatty acids, liquid mono-, di- and triglyceride mixtures based on C6-C18 fatty acids, esters of C6-C22 fatty alcohols and/or Guerbet alcohols with aromatic carboxylic acids, such as benzoic acid, esters of dicarboxylic acids with polyols containing 2 to 10 carbon atoms and 2 to 6 hydroxyl groups, vegetable oils, branched primary alcohols, substituted cyclohexanes, linear and branched C6-C22 fatty alcohol carbonates such as dicaprylyl carbonate (Cetiol®CC), Guerbet carbonates based on fatty alcohols containing 6 to 18, preferably 8 to 10, carbon atoms, esters of benzoic acid with linear and/or branched C6 to C22 alcohols (for example Finsolv® TN), linear or branched, symmetrical or nonsymmetrical dialkyl ethers containing 6 to 22 carbon atoms per alkyl group such as dicaprylyl ether (Cetiol® OE), ring opening products of epoxidized fatty acid esters with polyols and hydrocarbons or mixtures thereof.

Antioxidants are able to inhibit or prevent the undesired changes in the compositions to be protected caused by oxygen effects and other oxidative processes. The effect of the antioxidants consists in most cases in them acting as free-radical scavengers for the free radicals which arise during autoxidation.

In some embodiment, the antioxidant is selected from, but not limited to, amino acids and derivatives thereof (for example glycine, alanine, arginine, serine, threonine, histidine, tyrosine, tryptophan), imidazoles and derivatives thereof (e.g. urocanic acid), peptides and derivatives thereof (such as D, L-carnosine, D-carnosine, L-carnosine, β -Alanyl-L-histidine), carotenoids and carotenes or

derivatives thereof (e.g. alpha-carotene, beta-carotene, lycopene, lutein),
 chlorogenic acid and derivatives thereof, lipoic acid and derivatives thereof (for
 example dihydrolipoic acid), auro-thioglucose, propylthiouracil and other thiols
 and salts thereof (for example thioredoxin, glutathione, cysteine, cystine,
 5 cystamine and the glycosyl, N-acetyl, methyl, ethyl, propyl, amyl, butyl and
 lauryl, palmitoyl, oleyl, gamma-linoleyl, cholesteryl and glyceryl esters thereof),
 dilauryl thiodipropionate, distearyl thiodipropionate, thiodipropionic acid and
 derivatives thereof (esters, ethers, peptides, lipids, nucleotides, nucleosides and
 salts), sulfoximine compounds (for example buthionine sulfoximines,
 10 homocysteine sulfoximine, buthionine sulfones, penta-, hexa-, heptathionine
 sulfoximine), (metal) chelating agents (e.g. alpha-hydroxy fatty acids, palmitic
 acid, phytic acid, lactoferrin), alpha-hydroxy acids (for example citric acid, lactic
 acid, malic acid), humic acid, bile acid, bile extracts, bilirubin, biliverdin, boldin
 (=alkaloid from the plant *Peumus boldus*, boldo extract, EDTA, EGTA and
 15 derivatives thereof, unsaturated fatty acids and derivatives thereof (e.g.
 gamma-linolenic acid, linoleic acid, oleic acid), folic acid and derivatives thereof,
 ubiquinone and ubiquinol and derivatives thereof, vitamin C and derivatives (for
 example ascorbyl palmitate, Mg ascorbyl phosphate, ascorbyl acetate),
 tocopherols and derivatives (for example vitamin E acetate), vitamin A and
 20 derivatives (for example vitamin A palmitate), coniferyl benzoate of gum
 benzoin, rutic acid and derivatives thereof, alpha-glycosylrutin, ferulic acid,
 furfurylidene-glucitol, butylhydroxytoluene (BHT), butylhydroxyanisole (BHA),
 nordihydroguaiacic acid, nordihydroguaiaretic acid, trihydroxybutyrophenone,
 uric acid and derivatives thereof, mannose and derivatives thereof, superoxide
 25 dismutase, zinc and derivatives thereof (for example ZnO, ZnSO₄), selenium
 and derivatives thereof (for example selenomethionine) and stilbenes and
 derivatives thereof (e.g. stilbene oxide, trans-stilbene oxide) and mixtures of
 two or more of the aforementioned. The anti-oxidant may be selected from
 Tinogard® TT (BASF), Tinogard® Q (BASF), Tocopherol (including its isomers),
 30 2,6- bis(1,1-dimethylethyl)-4-methylphenol (BHT, CAS 128-37-0) and related
 phenols, hydroquinones.

In some embodiments, the antioxidants is characterised by a concentration of

about 0.1 wt% to about 20 wt% relative to the composition. In other
embodiments, the concentration is about 0.1 wt% to about 18 wt%, about 0.1
wt% to about 16 wt%, about 0.1 wt% to about 14 wt%, about 0.1 wt% to about
12 wt%, about 0.1 wt% to about 10 wt%, about 0.1 wt% to about 8 wt%, about
5 0.1 wt% to about 6 wt%, about 0.1 wt% to about 4 wt%, or about 0.1 wt% to
about 2 wt%.

Deodorizing compositions (deodorants and antiperspirants) counteract, mask or
eliminate body odors. Body odors are formed through the action of skin bacteria
10 on apocrine perspiration which results in the formation of unpleasant smelling
degradation products.

In some embodiments, the deodorant-active agent is selected from
antiperspirants, esterase inhibitors and antibacterial agents. Suitable
15 antiperspirant are, but not limited to, salts of aluminum, zirconium or zinc.
Examples are aluminum chloride, aluminum chlorohydrate, aluminum
dichlorohydrate, aluminum sesquichlorohydrate and complex compounds
thereof, for example with 1,2-propylene glycol, aluminum hydroxyallantoinate,
aluminum chloride tartrate, aluminum zirconium trichlorohydrate, aluminum
20 zirconium tetrachlorohydrate, aluminum zirconium pentachlorohydrate and
complex compounds thereof, for example with amino acids, such as glycine.

Where perspiration is present in the underarm region, extracellular enzymes-
esterases, mainly proteases and/or lipases are formed by bacteria and split the
25 esters present in the perspiration, releasing odors in the process. Suitable
esterase inhibitors are for example trialkyl citrates, such as trimethyl citrate,
tripropyl citrate, triisopropyl citrate, tributyl citrate and, in particular, triethyl
citrate. Esterase inhibitors inhibit enzyme activity and thus reduce odor
formation. The free acid is probably released by the cleavage of the citric acid
30 ester and reduces the pH value of the skin to such an extent that the enzymes
are inactivated by acylation. Other esterase inhibitors are sterol sulfates or
phosphates such as, forexample, lanosterol, cholesterol, campesterol,
stigmasterol and sitosterol sulfate or phosphate, dicarboxylic acids and esters

thereof, for example glutaric acid, glutaric acid monoethyl ester, glutaric acid diethyl ester, adipic acid, adipic acid monoethyl ester, adipic acid diethyl ester, malonic acid and malonic acid diethyl ester, hydroxycarboxylic acids and esters thereof, for example citric acid, malic acid, tartaric acid or tartaric acid diethyl ester, and zinc glycinate.

In some embodiments, the deodorants and antiperspirants is characterised by a concentration of about 0.1 wt% to about 20 wt% relative to the composition. In other embodiments, the concentration is about 0.1 wt% to about 18 wt%,
 10 about 0.1 wt% to about 16 wt%, about 0.1 wt% to about 14 wt%, about 0.1 wt% to about 12 wt%, about 0.1 wt% to about 10 wt%, about 0.1 wt% to about 8 wt%, about 0.1 wt% to about 6 wt%, about 0.1 wt% to about 4 wt%, or about 0.1 wt% to about 2 wt%.

15 The term "anti-bacterial agents" as used herein encompasses substances which have bactericidal and/or bacteriostatic properties. Typically these substances act against gram-positive bacteria such as, for example, 4-hydroxybenzoic acid and salts and esters thereof, N-(4-chlorophenyl)-N'-(3,4-dichlorophenyl)-urea, 2,4,4'-trichloro-2'-hydroxydiphenylether (triclosan), 4-chloro-3,5-
 20 dimethylphenol, 2,2'-methylene-bis-(6-bromo-4-chlorophenol), 3-methyl-4-(1-methylethyl)-phenol, 2-benzyl-4-chlorophenol, 3-(4-chlorophenoxy)-propane-1,2-diol, 3-iodo-2-propinyl butyl carbamate, chlorhexidine, 3,4,4'-trichlorocarbanilide (TTC), phenoxyethanol, glycerol monocaprato, glycerol monocaprylate, glycerol monolaurate (GML), diglycerol monocaprato (DMC),
 25 salicylic acid-N-alkylamides such as, for example, salicylic acid-n-octyl amide or salicylic acid-n-decyl amide.

In some embodiments, the antibacterial agent is selected from chitosan, phenoxyethanol, 5-chloro-2-(2,4-dichlorophenoxy)-phenol, 4-hydroxybenzoic
 30 acid and salts and esters thereof, N-(4-chlorophenyl)-N'-(3,4-dichlorophenyl)-urea, 2,4,4'-trichloro-2'-hydroxydiphenylether (triclosan), 4-chloro-3,5-dimethyl phenol, 2,2'-methylene-bis-(6-bromo-4-chlorophenol), 3-methyl-4-(1-methylethyl)-phenol, 2-benzyl-4-chlorophenol, 3-(4-chlorophenoxy)-

propane-1,2-diol, 3-iodo-2-propinyl butyl carbamate, chlorhexidine, 3,4,4'-trichlorocarbaniide (TTC), phenoxyethanol, glycerol monocaprates, glycerol monocaprylate, glycerol monolaurate (GML), diglycerol monocaprates (DMC), salicylic acid-N-alkylamides and mixtures of two or more of the aforementioned.

5

In some embodiments, the antibacterial agent is characterised by a concentration of about 0.1 wt% to about 20 wt% relative to the composition. In other embodiments, the concentration is about 0.1 wt% to about 18 wt%, about 0.1 wt% to about 16 wt%, about 0.1 wt% to about 14 wt%, about 0.1 wt% to about 12 wt%, about 0.1 wt% to about 10 wt%, about 0.1 wt% to about 8 wt%, about 0.1 wt% to about 6 wt%, about 0.1 wt% to about 4 wt%, or about 0.1 wt% to about 2 wt%.

In some embodiments, the composition comprises a surfactant. The surfactant may be selected from anionic, non-ionic, cationic, amphoteric, zwitterionic surfactants and mixtures of two or more of the aforementioned.

In some embodiments, the surfactant is characterised by a concentration of about 0.1 wt% to about 20 wt% relative to the composition. In other embodiments, the concentration is about 0.1 wt% to about 18 wt%, about 0.1 wt% to about 16 wt%, about 0.1 wt% to about 14 wt%, about 0.1 wt% to about 12 wt%, about 0.1 wt% to about 10 wt%, about 0.1 wt% to about 8 wt%, about 0.1 wt% to about 6 wt%, about 0.1 wt% to about 4 wt%, or about 0.1 wt% to about 2 wt%.

25

Typical examples of nonionic surfactants are fatty alcohol polyglycol ethers, alkylphenol, polyglycol ethers, fatty acid polyglycol esters, fatty acid amide polyglycol ethers, fatty amine polyglycol ethers, alkoxylated triglycerides, mixed ethers and mixed formals, optionally partly oxidized alk(en)yl oligoglycosides or glucuronic acid derivatives, fatty acid-N-alkyl glucamides, protein hydrolysates (particularly wheat-based vegetable products), polyol, fatty acid esters, sugar esters, sorbitan esters, polysorbates and amine oxides. If the nonionic surfactants contain polyglycol ether chains, they may have a conventional

homolog distribution, although they preferably have a narrow range homolog distribution.

Zwitterionic surfactants are surface-active compounds which contain at least one quaternary ammonium group and at least one COO(-) or SO₃(-) group in the molecule. Particularly suitable zwitterionic surfactants are the so-called betaines, such as the N-alkyl-N,N-dimethyl ammonium glycinate, for example, cocoalkyl dimethyl ammonium glycinate, N-acylaminoethyl-N,N-dimethyl ammonium glycinate, for example, cocoacylaminoethyl dimethyl ammonium glycinate, and 2-alkyl-3-carboxymethyl-3-hydroxyethyl imidazolines, containing 8 to 18 carbon atoms in the alkyl or acyl group, and cocoacylaminoethyl hydroxyethyl carboxymethyl glycinate. The fatty acid amide derivative known under the CTFA name of Cocamidopropyl Betaine may be preferred.

Ampholytic surfactants are also suitable, particularly as co-surfactants. Ampholytic surfactants are surface active compounds which, in addition to a C₈ to C₁₈ alkyl or acyl group, contain at least one free amino group and at least one -COOH or -SO₃H group in the molecule and which are capable of forming inner salts. Examples of suitable ampholytic surfactants are N-alkyl glycines, N-alkyl propionic acids, N-alkylaminobutyric acids, N-alkyliminodipropionic acids, N-hydroxyethyl-N-alkylamidopropyl glycines, N-alkyl taurines, N-alkyl sarcosines, 2-alkylaminopropionic acids and alkylaminoacetic acids containing around 8 to 18 carbon atoms in the alkyl group. Particularly preferred ampholytic surfactants are N-cocoalk-ylaminopropionate, cocoacylaminoethyl aminopropionate and acyl sarcosine.

Anionic surfactants are characterized by a water-solubilizing anionic group such as, for example, a carboxylate, sulfate, sulfonate or phosphate group and a lipophilic group. Dermatologically safe anionic surfactants are known to the practitioner in large numbers from relevant textbooks and are commercially available. They are, in particular, alkyl sulfates in the form of their alkali metal, ammonium or alkanolammonium salts, alkylether sulfates, alkylether

carboxylates, acyl isethionates, acyl sarcosinates, acyl taurines containing linear C12-C18 alkyl or acyl groups and sulfosuccinates and acyl glutamates in the form of their alkali metal or ammonium salts.

- 5 Suitable cationic surfactants may be quaternary ammonium compounds, for example ammonium halides, more especially chlorides and bromides, such as alkyl trimethyl ammonium chlorides, dialkyl dimethyl ammonium chlorides and trialkyl methyl ammonium chlorides, for example, cetyl trimethyl ammonium chloride, stearyl trimethyl ammonium chloride, distearyl dimethyl ammonium chloride, lauryl dimethyl ammonium chloride, lauryl dimethyl benzyl ammonium chloride and tricetyl methyl ammonium chloride. In addition, the readily biodegradable quaternary ester compounds, such as, for example, the dialkyl ammonium methosulfates and methyl hydroxyalkyl dialkylalkoxyalkyl ammonium methosulfates marketed under the name of Stepanitex and the corresponding products of the Dehyquart® series, may be used as cationic surfactants. "Esterquats" are generally understood to be quaternized fatty acid triethanolamine ester salts. They can provide the compositions with particular softness.
- 10
- 15
- 20 The composition may be a perfume composition, cosmetic composition, body care composition, hygiene article, cleaning composition, textile detergent composition, composition for scent dispenser, food, food supplement, pharmaceutical composition and crop protection composition.
- 25 The perfume composition may be selected from fine fragrances, air fresheners in liquid form, gel-like form or a form applied to a solid carrier, aerosol sprays, scented cleaners, perfume candles and oils, such as lamp oils or oils for massage.
- 30 Example for fine fragrances are perfume extracts, Eau de Parfums, Eau de Toilettes, Eau de Colognes, Eau de Solide and Extrait Parfum.

Body care compositions include cosmetic compositions and products for oral and

dental hygiene, and may be selected from after-shaves, pre-shave products, splash colognes, solid and liquid soaps, shower gels, shampoos, shaving soaps, shaving foams, bath oils, cosmetic emulsions of the oil-in-water type, of the water-in-oil type and of the water-in-oil-in-water type, such as e.g. skin creams
5 and lotions, face creams and lotions, sunscreen creams and lotions, aftersun creams and lotions, hand creams and lotions, foot creams and lotions, hair removal creams and lotions, after-shave creams and lotions, tanning creams and lotions, hair care products such as e.g. hairsprays, hair gels, setting hair lotions, hair conditioners, hair shampoo, permanent and semi-permanent hair
10 colorants, hair shaping compositions such as cold waves and hair smoothing compositions, hair tonics, hair creams and hair lotions, deodorants and antiperspirants such as e.g. underarm sprays, roll-ons, deodorant sticks and deodorant creams, products of decorative cosmetics such as e.g. eye-liners, eye-shadows, nail varnishes, make-ups, lipsticks and mascara, and products for
15 oral and dental hygiene, such as toothpaste, dental floss, mouth wash, breath fresheners, dental foam, dental gels and dental strips.

Hygiene articles may be selected from joss sticks, insecticides, repellents, propellants, rust removers, perfumed freshening wipes, armpit pads, baby
20 diapers, sanitary towels, toilet paper, cosmetic wipes, pocket tissues, dishwasher and deodorizer.

Cleaning compositions, such as e.g. cleaners for solid surfaces, may be selected from perfumed acidic, alkaline and neutral cleaners, such as e.g. floor cleaners,
25 window cleaners, dishwashing compositions both for handwashing and machine washing use, bath and sanitary cleaners, scouring milk, solid and liquid toilet cleaners, powder and foam carpet cleaners, waxes and polishes such as furniture polishes, floor waxes, shoe creams, disinfectants, surface disinfectants and sanitary cleaners, brake cleaners, pipe cleaners, limescale removers, grill
30 and oven cleaners, algae and moss removers, mold removers, facade cleaners.

Textile detergent compositions may be selected from liquid detergents, powder detergents, laundry pretreatments such as bleaches, soaking agents and stain

removers, fabric softeners, washing soaps, washing tablets.

Food means a raw, cooked, or processed edible substance, ice, beverage or ingredient used or intended for use in whole or in part for human consumption,
5 or chewing gum, gummies, jellies, and confectionaries.

A food supplement is a product intended for ingestion that contains a dietary ingredient intended to add further nutritional value to the diet. A dietary ingredient may be one, or any combination, of the following substances: a
10 vitamin, a mineral, an herb or other botanical, an amino acid, a dietary substance for use by people to supplement the diet by increasing the total dietary intake, a concentrate, metabolite, constituent, or extract. Food supplements may be found in many forms such as tablets, capsules, soft gels, gel caps, liquids, or powders.

15 Pharmaceutical compositions comprise compositions which are intended for use in the diagnosis, cure, mitigation, treatment, or prevention of disease as well as articles (other than food) intended to affect the structure or any function of the body of man or other animals.

20 Crop protection compositions comprise compositions which are intended for the managing of plant diseases, weeds and other pests (both vertebrate and invertebrate) that damage agricultural crops and forestry.

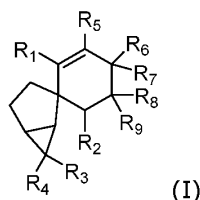
25 In some embodiment, the composition further comprises at least one auxiliary agent selected from the group consisting of preservatives, abrasives, anti-acne agents, agents to combat skin aging, anti-cellulite agents, antidandruff agents, anti-inflammatory agents, irritation-preventing agents, irritation-alleviating agents, astringents, sweat inhibiting agents, antiseptics, anti-statics, binders,
30 buffers, carrier materials, chelating agents, cell stimulants, care agents, hair removal agents, emulsifiers, enzymes, essential oils, fibers, film formers, fixatives, foam formers, foam stabilizers, substances for preventing foaming, foam boosters, fungicides, gelling agents, gel-forming agents, hair care agents,

hair shaping agents, hair smoothing agents, moisture-donating agents, moisturizing substances, humectant substances, bleaching agents, strengthening agents, stain removal agents, optical brighteners, impregnating agents, soil repellents, friction-reducing agents, lubricants, moisturizing
 5 creams, ointments, opacifiers, plasticizers, covering agents, polish, shine agents, polymers, powders, proteins, refatting agents, exfoliating agents, silicones, skin-calming agents, skin cleansing agents, skin care agents, skin-healing agents, skin lightening agents, skin-protective agents, skin-softening agents, cooling agents, skin-cooling agents, warming agents, skin-warming
 10 agents, stabilizers, UV-absorbent agents, UV filters, fabric softeners, suspending agents, skin-tanning agents, thickeners, vitamins, waxes, fats, phospholipids, saturated fatty acids, mono- or polyunsaturated fatty acids, α -hydroxy acids, polyhydroxy fatty acids, liquefiers, dyes, color-protection agents, pigments, anti-corrosives, polyols, electrolytes and silicone derivatives.

15

The present disclosure also provides a method of formulating a composition, comprising:

adding a compound of Formula (I) or a salt, solvate or stereoisomer thereof:



20 wherein

R_1 , R_2 , R_3 and R_4 are independently selected from H, oxo, optionally substituted alkyl, optionally substituted alkenyl; and

R_5 , R_6 , R_7 , R_8 and R_9 are independently selected from H, oxo, optionally substituted alkyl, optionally substituted alkenyl;

25 wherein the compound of Formula (I) is characterised by a concentration of at least 80 ppm relative to the composition.

The present disclosure also provides a method of providing an aroma to a composition, comprising a step of adding a compound of Formula (I) to the

composition, wherein the compound of Formula (I) is characterised by a concentration of at least 80 ppm relative to the composition.

The present disclosure also provides a use of a compound of Formula (I) to
5 impart an aroma, wherein the compound of Formula (I) is added such that its final concentration is at least 80 ppm.

Examples

Purification of compound 1.

10 Compound 1 was produced according to Cheong et al. ACS Chem. Biol. 2023, 18, 134–140, the reference of which is incorporated herein. The two sesquiterpene synthases (STS) enzymes LdSTS7 and LdSTS11 are SEQ 1 and SEQ 2 respectively. The extracted terpenoids were analyzed using GC-MS to determine the level of the terpenoid products along with 10 mg/L of
15 caryophyllene standard. The calculated yield of the product mixture was estimated at ~80 mg/L.

The isolated terpene sample contained primarily a mixture of the major 1 and minor product 2 (ca. 2:1 peak area based on GC-TIC, Figure 1A) with trace
20 amounts of product 3. Due to the volatile nature of the compounds, further attempts to purify the components by flash column chromatography or preparative thin-layer chromatography (TLC) were unsuccessful. The GC-MS spectra of both products had $m/z = 204$, which was corroborated by LC-HRMS, suggesting that the products could be structural isomers with very similar
25 physical characteristics. The IR spectrum did not show the presence of any hydroxy groups ($2500\text{--}3600\text{ cm}^{-1}$). Combining elemental analysis (absence of nitrogen group) with the chemical formula ($\text{C}_{15}\text{H}_{24}$), a sesquiterpene hydrocarbon with 4 degrees of unsaturation is proposed.

30 NMR Analysis of the LdSTS7 Terpene Products.

Initial 1D and 2D NMR experiments revealed significant peak overlaps as well as low signal intensity due to limited sample quantity. Thus, selective and semiselective 1D and 2D NMR experiments were employed for *de novo* structure

elucidation to resolve and rigorously identify individual signals from each component in the volatile colorless oil mixture while concurrently obtaining accurate J-couplings and ¹H multiplicities. Initial attempts at separating the compounds from LdSTS7 by flash column chromatography were met with very
5 limited success, and only managed to improve the ratio of compounds 1/2 slightly from about 2:1 (by GC-MS) to about 4:1 (by NMR). The postchromatography outcome (with 4:1 ratio) was used subsequently for NMR structure elucidation.

10 Briefly, 1D selective TOCSY experiments identified two well-defined spin systems for the major compound 1, leaving two CH₃ singlets and two quaternary carbons based on the chemical formula (Figure 2B). The identities of the spin systems were confirmed by 2D HSQC experiments. The connectivities of the fragments were obtained by 2D semiselective HMBC experiments, revealing the
15 main spiro[4.5]dec-6-ene skeleton bearing a key spiro center, as well as a gem-dimethylcyclopropyl motif (Figure 2C). 1D selective NOESY experiments then identified protons that were close in space (Figure 2D), thus confirming the relative stereochemistry about the 4 stereogenic centers and affording the final structure of compound 1.

20

The remaining minor compounds 2 and 3 (Figure 2A) were identified to be 9-aristolene (2) and 1-aristolene (3) based on similar de novo structural elucidation from (semiselective) 1D and 2D NMR experiments, followed by subsequent verification after a structure search (Reaxys) and comparison of ¹H
25 and ¹³C NMR chemical shifts from literature data.

Analysis on GC-QTOF-O (DB-5 column)

Samples are dissolved in Dichloromethane, 10ppm and injected using an aliquot volume of 5ul under splitless mode. The retention time (RT) of compound 1 is
30 14.1 min, retention index (RI) is 1465. No smell was identified (based on 2 analysts).

Analysis on GC-QTOF-O (Wax column)

Samples are dissolved in Dichloromethane, 100ppm and injected using an aliquot volume of 1ul under splitless mode. The retention time (RT) of compound 1 is 11.6 min, RI is 1417. The odour description (based on 2 analysts) is:

#1: Earthy, woody : novel pirobicyclo[3.1.0]terpene

5 #2: Woody, green : 9-aristolene

#3: No odour detected : 1-aristolene

Odour description of the sample (mixture) from the bottle:

Earthy, medicinal, woody

10

MATERIALS AND METHODS

Gas ChromatographyMass Spectroscopy (GC-MS) Analysis of Terpenoids.

GC-MS was used for the detection and quantification of terpenes:

For the large-scale production (400 mL) and product purification, the products

15 of LdSTS7 were determined with an Agilent Intuvo 9000 equipped with an

Agilent 5977B MSD. For each extracted fraction, 10 µL of sample was diluted 20

times with 190 µL hexane, then 1 µL was injected onto the Agilent DB-WAX

Ultra Inert GC column (30 m × 250 µm × 0.25 µm). The split ratio of 20:1 was

set at 250 °C. The oven temperature was initially held at 100 °C for 1 min and

20 increased to 150 °C at a rate of 50 °C/min and further increased to 220 °C at a

rate of 15 °C/min. Finally, the temperature was increased to 240 °C at a rate

of 50 °C/min and held for 2 min. Mass spectrometer was operated in EI mode

with scanning after a 3 min solvent delay (ranging from 50 to 350 m/z). To

calculate the relative yield of the terpene products, caryophyllene (10 mg/L)

25 was used as an internal standard. The detected peaks were predicted through

literature data in the NIST database.

Nuclear Magnetic Resonance (NMR) Spectroscopy.

All spectra were acquired on a Bruker AV Neo 400 MHz spectrometer equipped with a RT 5 mm

30 z-gradient BBFO probe or on a Bruker AVIII 400 MHz spectrometer equipped

with a 5 mm z-gradient ¹³C/¹H/²H DCH observe cryoprobe. All NMR

experiments were performed without sample rotation at 298 K in CDCl₃. The

following selective refocusing pulses were used to select desired frequencies

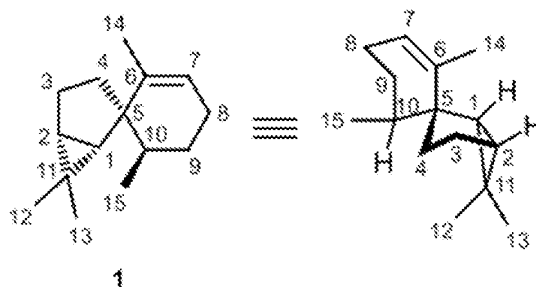
through carrier-shift: Gaus1_180r.1000 (80 or 120 ms) for 1D TOCSY, CLIP-COSY and NOESY, and Q3_surbop.1 (815 μ s) for 2D band-selective HSQC and HMBC. For clarity, all 1D TOCSY, CLIP-COSY, and NOESY experiments in this paper refer to their selective variants that employ selective refocusing
 5 (excitation sculpting via spfge).

Data acquisition was performed using the software Bruker TopSpin 4.0.9 using pulse sequences obtained therein. Initial data processing was performed using Topspin 4.0.9, then further data processing, spectral analysis, and spectra
 10 generation were performed using Mestrenova 12.0.2 unless otherwise stated. Baseline correction for 1D and 2D spectra was not used unless otherwise stated. Forward linear prediction on F1 dimension was used for all 2D spectra (except JRES). JRES data was processed with 45° tilt and J-symmetrization with sensitivity enhancement (Mestrenova).

15

Compound 1

rel-(1S,2S,5R,6'R)-2',6,6,6'-Tetramethylspiro[bicyclo[3.1.0]hexane-2,1'-cyclohexan]-2'-ene



20 ^1H NMR (400.1 MHz, CDCl_3) δ 5.209 (1H, ddquint, J = 5.1, 2.5, 1.3 Hz, C7H), 2.040 (1H, dddquint, J = 17.8, 12.5, 6.0, 2.3 Hz, C8H_AH_B), 2.012 (1H, dddd, J = 13.4, 11.1, 8.8, 6.1 Hz, C3H_AH_B), 1.866 (1H, ddd, J = 14.1, 10.8, 1.6 Hz, C4H_AH_B), 1.854 (1H, qt, J = 7.0, 3.5 Hz, C10H), 1.809 (1H, dtquint, J = 17.8, 5.8, 1.5 Hz, C8H_AH_B), 1.734 (3H, dt, J = 2.8, 1.4 Hz, C14H₃), 1.727 (1H, ddd,
 25 J = 13.5, 9.9, 2.0 Hz, C3H_AH_B), 1.594 (1H, tdd, J = 12.5, 6.0, 3.4 Hz, C9H_AH_B), 1.484 (1H, dt, J = 13.8, 9.3 Hz, C4H_AH_B), 1.448 (1H, dddt, J = 12.7, 6.1, 3.4,

1.4 Hz, C9H_AH_B), 1.192 (1H, t, J = 6.4 Hz, C2H), 1.165 (3H, s, C12H₃), 1.018 (3H, s, C13H₃), 1.001 (3H, d, J = 7.1 Hz, C15H₃), 0.861 (1H, d, J = 6.6 Hz, C1H).

5 ¹³C{¹H} NMR (100.6 MHz, CDCl₃) δ 141.35 (C6), 118.35 (C7), 51.43 (C5), 43.40 (C4H₂), 39.08 (C1H), 36.69 (C10H), 32.36 (C2H), 29.01 (C13H₃), 27.02 (C3H₂), 26.88 (C9H₂), 20.81 (C8H₂), 20.66 (C14H₃), 20.15 (C11), 17.19 (C12H₃), 16.46 (C15H₃).

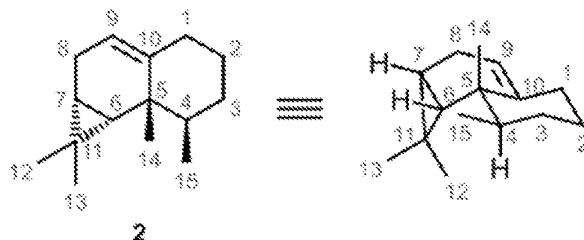
10 FT-IR (mixture, neat) 3000, 2963, 2867, 1456, 1374, 1203, 1124, 1030, 993, 954, 891, 813, 791, 621 cm⁻¹.

HRMS (mixture, ESI⁺) calcd. for C₁₅H₂₅ m/z (M⁺H)⁺: 205.19508, found: 205.1970.

15

9-Aristolene (2)

rel-(1aR,7R,7aR,7bS)-1,1,7,7a-Tetramethyl-1a,2,3,5,6,7,7a,7b-octahydro-1H-cyclopropa[a]-naphthalene



20 ¹H NMR (400.1 MHz, CDCl₃) δ 5.113 (1H, dq, J = 4.4, 2.5 Hz, C9H), 2.328 (1H, dddd, J = 18.8, 7.2, 4.3, 2.9 Hz, C8H_AH_B), 2.202 (1H, dddd, J = 15.7, 13.1, 4.3, 2.0 Hz, C1H_AH_B), 2.064 (1H, ddd, J = 18.8, 4.4, 2.1 Hz, C8H_AH_B), 1.996 (1H, ddt, J = 13.8, 4.2, 2.2 Hz, C1H_AH_B), 1.688 (1H, ddq, J = 11.9, 4.9, 2.5 Hz, C2H_AH_B), 1.627 (1H, dd, J = 11.6, 7.3 Hz, C4H), 1.532 – 1.432 (1H, m, C3H_AH_B),
 25 1.360 (1H, qd, J = 12.6, 3.1 Hz, C3H_AH_B), 1.263 (1H, qt, J = 12.9, 4.0 Hz, C2H_AH_B), 1.105 (3H, s, C12H₃), 1.073 (3H, s, C14H₃), 1.049 (3H, s, C13H₃),

0.963 (3H, d, $J = 6.8$ Hz, C15H₃), 0.781 (1H, dd, $J = 9.4, 7.1$ Hz, C7H), 0.629 (1H, d, $J = 9.4$ Hz, C6H).

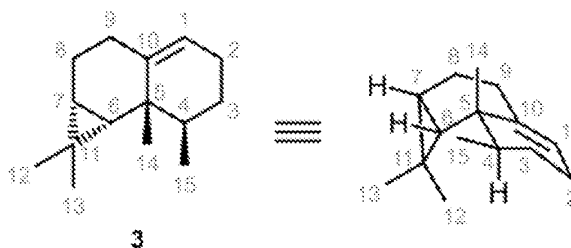
¹³C{¹H} NMR (100.6 MHz, CDCl₃) δ 141.64 (C10), 118.30 (C9H), 37.79 (C4H),
 5 36.75 (C5), 33.01 (C1H₂), 32.05 (C6H), 31.38 (C3H₂), 29.91 (C12H₃), 27.21 (C2H₂), 21.76 (C8H₂), 21.43 (C14H₃), 19.21 (C7H), 17.93 (C11), 16.00 (C15H₃), 15.76 (C13H₃).

The NMR data are consistent with those from literature.

10

1-Aristolene (3)

rel-(1aR,7R,7aR,7bS)-1,1,7,7a-Tetramethyl-1a,2,4,5,6,7,7a,7b-octahydro-1H-cyclopropa[a]-naphthalene Also known as: Caralene, β -Gurjurenene



15 ¹H NMR (400.1 MHz, CDCl₃) δ 5.266 (1H, dt, $J = 4.6, 2.3$ Hz, C1H), 2.314 – 2.179 (1H, m, C9H_AH_B), 2.035 – 1.917 (2H, m, C2H₂), 1.997 (1H, dddd, $J = 14.1, 9.8, 7.1, 1.5$ Hz, C8H_AH_B), 1.770 (1H, ddq, $J = 10.7, 6.7, 4.4$ Hz, C4H), 1.761 (1H, ddd, $J = 13.0, 5.8, 1.4$ Hz, C9H_AH_B), 1.496 – 1.386 (2H, m, C3H₂), 1.415 (1H, tdd, $J = 13.8, 5.8, 3.5$ Hz, C8H_AH_B), 1.092 (3H, s, C14H₃), 1.039
 20 (3H, s, C12H₃), 1.004 (3H, s, C13H₃), 0.993 (3H, d, $J = 6.9$ Hz, C15H₃), 0.762 (1H, td, $J = 9.6, 3.6$ Hz, C7H), 0.581 (1H, d, $J = 9.1$ Hz, C6H).

¹³C{¹H} NMR (100.6 MHz, CDCl₃) δ 144.18 (C10), 120.32 (C1H), 36.79 (C5), 36.69 (C4H), 33.49 (C6H), 29.94 (C9H₂), 29.88 (C12H₃), 27.22 (C3H₂), 25.71
 25 (C2H₂), 22.99 (C14H₃), 20.83 (C8H₂), 19.59 (C7H), 18.52 (C11), 16.50 (C13H₃), 16.10 (C15H₃).

The NMR data are consistent with those from literature. Assignments are based on comparison with literature values.

5 It will be appreciated that many further modifications and permutations of various aspects of the described embodiments are possible. Accordingly, the described aspects are intended to embrace all such alterations, modifications, and variations that fall within the spirit and scope of the appended claims.

10 Throughout this specification and the claims which follow, unless the context requires otherwise, the word "comprise", and variations such as "comprises" and "comprising", will be understood to imply the inclusion of a stated integer or step or group of integers or steps but not the exclusion of any other integer or step or group of integers or steps.

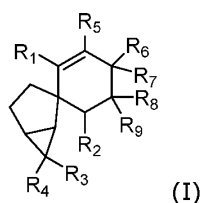
15 Throughout this specification and the claims which follow, unless the context requires otherwise, the phrase "consisting essentially of", and variations such as "consists essentially of" will be understood to indicate that the recited element(s) is/are essential i.e. necessary elements of the invention. The phrase allows for the presence of other non-recited elements which do not materially
20 affect the characteristics of the invention but excludes additional unspecified elements which would affect the basic and novel characteristics of the method defined.

25 The reference in this specification to any prior publication (or information derived from it), or to any matter which is known, is not, and should not be taken as an acknowledgment or admission or any form of suggestion that that prior publication (or information derived from it) or known matter forms part of the common general knowledge in the field of endeavour to which this specification relates.

30

Claims

1. A composition, comprising:
a compound of Formula (I) or a salt, solvate or stereoisomer thereof:



5

wherein

R₁, R₂, R₃ and R₄ are independently selected from H, oxo, optionally substituted alkyl, optionally substituted alkenyl; and

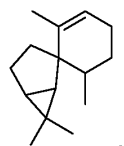
10 R₅, R₆, R₇, R₈ and R₉ are independently selected from H, oxo, optionally substituted alkyl, optionally substituted alkenyl;

wherein the compound of Formula (I) is characterised by a concentration of at least 80 ppm relative to the composition.

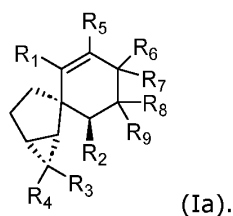
2. The composition according to claim 1, wherein R₁, R₂, R₃ and R₄ are
15 independently optionally substituted C₁-C₄ alkyl.

3. The composition according to claim 1 or 2, wherein R₅, R₆, R₇, R₈ and R₉ are independently selected from H, or optionally substituted C₁-C₄ alkyl.

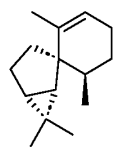
20 4. The composition according to any one of claims 1 to 3, wherein the compound of Formula (I) is



5. The composition according to any one of claims 1 to 4, wherein the
25 compound of Formula (I) is a compound of Formula (Ia):



6. The composition according to any one of claims 1 to 5, wherein the compound of Formula (I) is



5

7. The composition according to any one of claims 1 to 6, wherein the compound of Formula (I) is characterised by a concentration of at least 100 ppm relative to the composition.

10

8. The composition according to any one of claims 1 to 7, wherein the compound of Formula (I) is characterised by a woody and/or earthy scent.

9. The composition according to any one of claims 1 to 8, wherein the composition further comprises 9-aristolene.

15

10. The composition according to claim 9, wherein the 9-aristolene is characterised by a concentration of at least 20 ppm relative to the composition.

11. The composition according to any one of 1 to 10, wherein the composition further comprises 1-aristolene.

20

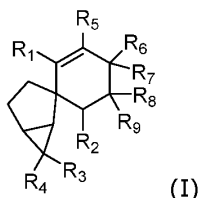
12. The composition according to claim 11, wherein the 1-aristolene is characterised by a concentration of less than 20 ppm relative to the composition.

25

13. The composition according to any one of claims 9 to 12, wherein the composition is characterised by a ratio of the compound of Formula (I) to 9-aristolene and 1-aristolene of about 2:1 to about 6:1.

5 14. The composition according to any one of claims 9 to 13, wherein the composition is characterised by a woody, earthy and medicinal scent.

15. A method of formulating a composition, comprising:
adding a compound of Formula (I) or a salt, solvate or stereoisomer thereof:



10

wherein

R₁, R₂, R₃ and R₄ are independently selected from H, oxo, optionally substituted alkyl, optionally substituted alkenyl; and

15 R₅, R₆, R₇, R₈ and R₉ are independently selected from H, oxo, optionally substituted alkyl, optionally substituted alkenyl;

wherein the compound of Formula (I) is characterised by a concentration of at least 80 ppm relative to the composition.

16. A method of providing an aroma to a composition, comprising a step of
20 adding a compound of Formula (I) to the composition, wherein the compound of Formula (I) is characterised by a concentration of at least 80 ppm relative to the composition.

17. Use of a compound of Formula (I) to impart an aroma, wherein the
25 compound of Formula (I) is added such that its final concentration is at least 80 ppm.