Title: DETECTION OF ANALYTES IN A DEFINED AREA OF THE BODY

Abstract: A method for determining qualitatively or quantitatively one or more analytes present in a defined area of the body of a subject characterized by the following steps: a) applying an adsorbent material to the defined area of the body of a subject, b) extracting the analyte from said area and removing the adsorbent material from the defined area of the body, c) desorbing the analyte from the adsorbent material, and d) detecting the analyte qualitatively or quantitatively. Moreover, the present invention relates to an adsorbent article or a patch suitable to be applied in this method and the use of the adsorbent article or the patch for determining qualitatively or quantitatively one or more analytes.
DETECTION OF ANALYTES IN A DEFINED AREA OF THE BODY

The invention relates to a method for determining qualitatively or quantitatively one or more analytes present in a defined area of the body of a subject; an adsorbent article or a patch suitable to be applied in this method and the use of the adsorbent article or the patch for determining qualitatively or quantitatively one or more analytes.

INTRODUCTION

The intensity and duration of perception of odor compounds during and after food consumption is influenced by a complex series of physiological and physical-chemical processes. Thereby, two key modes have to be distinguished, a) the immediate aroma impression when food is present in the oral cavity or is just swallowed and b) the prolonged retronasal aroma perception after swallowing, often called aftertaste or better "afterodor" or "aftersmell" when talking of odorants. For a detailed explanation of the physiological features, refer to (1). Odorous substances are found amongst very different substance classes such as esters, aldehydes, alcohols, thio-compounds, heteroaromatic or terpenic compounds and many more. Prolonged retronasal aroma perception, as it is perceived after complete swallowing of a food, must be induced by persistent odorants which are present in the oral cavity during a certain period. This means that they are adsorbed to oral mucosa as a kind of aroma reservoir and released there from continuously. This adsorption of odorants, as it has been previously shown to occur (1, 2), can be regarded as the only possible explanation for the persistence of odorous molecules after food consumption and for the development and/or duration of the so-called afterodor. Up to now, the premises for this phenomenon could not be fully elucidated. As discussed above, it has been shown that odorants are adsorbed to the oral mucosa. However, the subsequent release; which is an important prerequisite for their retronasal perception, has been proposed but could not be proofed. Generally; retronasal aroma perception of odorants released in the oral cavity is only possible when the velum-tongue border is opened. This can occur, for example, during talking, breathing through the mouth, swallowing of saliva or often just unconsciously at rest. To varying amount, this can result in a transfer of aroma-loaded air and/or
saliva into the pharynx depending on the type and extent of action performed. From the pharyngeal areas, the air is further transported by the tidal breath-flow into the nasal cavity and to the olfactory epithelium. This transfer can be enhanced by deliberate pumping actions performed with the velum, again a process which is often performed by people unconsciously e.g. during after consumption of a delightful meal.

As another aspect of the phenomenon, the influence of human salivary enzymes on the differences in persistence between odorants, apart from physicochemical parameters such as polarity and volatility, has been proposed (3, 4). Generally, it has been elucidated that saliva can act as an aroma extraction and transporting system by continuously extracting odorants from materials which are not swallowed, for example chewing gum. These compounds are then transferred during the swallowing process into the pharyngeal areas where they can be perceived retronasally as described in (1). Apart from the direct release into the buccal air phase, the same extraction process, that means a kind of “washing-out” effect, has been assumed for odorants which are adsorbed to the oral mucosa.

To proof the existence of these release processes after food consumption, the main goal of the present study was to develop a technique which allows the characterization of potent odorants released into the oral cavity even at extremely low concentrations from the oral mucosa or from films covering the mucosa like a kind of coating. This should be preferably achieved by a technique which allows intraoral application as deliberate expectoration of saliva samples might result in odor losses into the air phase or to sampling devices. Also, it might alter the natural saliva flow parameters as it is not easily achieved to collect even minor amounts of saliva from panelists. This would, consequently, lead to changes in intra-oral aroma release. On the other hand, a precisely defined starting point for sample collection within very narrow time frames is a inevitable prerequisite for the investigation of the mostly fast retronasal aroma changes after food consumption. Subsequent screening of the odor contribution of the respective odorants should be achieved by a odor-intensity based approach.

A very versatile and sensitive extraction technique for gaseous and liquid samples, which has been recently developed, is the stir bar sorptive extraction (SBSE) (5). In SBSE, a PDMS-coated stir bar is exposed for a certain extraction time to a certain
volume of sample either with or without preliminary application of derivatization techniques. After trapping of the analytes to the SBSE bars and removal of the matrix system, the analytes can be easily recovered via extraction or thermodesorption and analysed e.g. by gas chromatography or liquid chromatography in combination with the respective detector systems. Compared to other sorptive sample preparation techniques such as SPME, the SBSE has several advantages such as convenient handling, high extraction capacity, very low amounts of PDMS breakdown products and many more (6). Apart from environmental investigations such as pesticide analysis and several others (6, 7, 8), first applications of SBSE have been recently reported for the direct analysis of e.g. benzoic acid or dicarboximide fungicides in foods and beverages (9, 10), and also for the elucidation of biochemical pathways (11). Application of the system for the analysis of odorous compounds are still rare and focused on the direct analysis in the respective samples (12, 13, 14).

Combination with multidimensional gas chromatography using chiral chromatography systems allowed the assignment of the stereochemistry of aroma compounds in foods such as strawberries (15). In-vitro studies of e.g. biological markers, drugs, their metabolites or other artificial contaminants such as PCB have been just recently performed on body fluids such as sperm, blood and urine (16, 17). However, in-vivo applications and use in salivary environment have not been reported. Therefore, the aim of the present investigation was (i) to proof the capacity of the SBSE system in combination of high resolution gas chromatography-olfactometry (HRGC/O) for the detection of extremely low concentrated but potent odorants down to their threshold levels and (ii) the applicability of the system for intra-oral odor investigation. In this context, elucidation of the changes in the retronasally perceived aroma profiles with time was of key interest. Also, as the commonly used extraction parameters (30 min or more, etc.) were not feasible for intra-oral application.

Therefore, the third key goal was to proof the capacity of the system under optimized extraction conditions (e.g. a few minutes of extraction time, little sample volume) with respect to time-resolved retronasal aroma perception.
Summary of the Invention

The invention relates to a method for determining qualitatively or quantitatively one or more analytes present in a defined area of the body of a subject characterised by the following steps:

a) applying an adsorbent material to the defined area of the body of a subject,
b) extracting the analyte from said area and removing the adsorbent material from the defined area of the body,
c) desorbing the analyte from the adsorbent material, and
d) detecting the analyte qualitatively or quantitatively.

Preferably, steps a-d) are repeated at least once.
Preferably, the area of the body is the oral cavity, the nasal cavity, the vagina, the anal cavity, hair, or another area of the skin.

The invention further relates to a method where the area of the body is selected from mouth, nose, vagina, anal cavity, hair, especially head hair, or areas of the skin, including armpits.

Preferably, the following steps are conducted:

a) applying an adsorbent article to the defined area of the body from a living subject at predefined starting point
b) extracting the analyte for a defined period from said area and removing the adsorbent article from the defined area of the body
c) desorption of the analyte from the adsorbing material
d) detection of the analyte
e) optionally steps a-d) are carried out more than once where optionally the extraction period in b) may vary.

The invention further relates to a method as defined above where a composition comprising the analytes or a precursor thereof is administered to a subject prior to application of the adsorbent material.
In this case steps a-d) or all steps may be carried out more than once and the interval between administration of the composition and starting point a) may vary between every analyses.

In a further aspect of the invention the composition comprising the analytes or a precursor thereof is administered orally.

Furthermore the invention relates to a method as defined above where the adsorbent material or article is introduced into the mouth and extraction takes place within the mouth.

In a further aspect the composition is selected from food, beverage, or a matrix spiked with the analyte or a precursor, tobacco-ware or the smoke thereof.

In a further aspect the component comprising the analytes or a precursor thereof is administered topically. Preferably the composition is selected from fragrances, deodorants, antiperspirants, skin care products, cleansing products, decorative cosmetic products, pharmaceutically active topical preparations, and mixtures thereof; more preferably the composition is formulated as a medicament or cosmetic, perfume, skin care, hair-wash, deodorant, ointment, cream, sun cream, lotion, soap, shampoo, or other rinsing product.

The invention furthermore relates to a method as defined above where the composition comprising the analytes or a precursor thereof is administered topically, and the adsorbent material is applied to the skin and extraction takes place at the surface of the skin. Application of the adsorbent article may take place at an area different to where the administration of said composition took place or at the same area. In most cases the latter option is preferred.

In one aspect of the invention, the composition comprising the analyte or a precursor thereof is administered nasally, anally, or vaginally. Preferably, the adsorbent material is applied to the nasal cavity, vagina, or anal cavity, respectively, and extraction takes place at the nasal cavity, vagina or anal cavity, respectively.
Preferably the adsorbent material is selected from compounds of polydialkylsiloxanes, polyphenyleneoxides, divinylbenzene, polyacrylates, activated alumina, carbon black, carbon molecular sieve adsorbent resins, polyethylene glycols, diatomaceous earth based adsorbents and mixtures of two or more thereof. More preferably, it is selected from polydialkylsiloxanes, polyphenyleneoxide (Tenax®), divinylbenzene, carbowax/divinylbenzene, carboxen/PDMS, PDMS/divinylbenzene, carboxen/divinylbenzene, and polyacrylate. Polydialkylsiloxanes such as polydimethylsiloxane (PDMS), divinylbenzene, carbowax/divenylbenzene, carboxen/PDMS, PDMS/divenylbenzene, carboxen/divinylbenzene, polyacrylate are particularly preferred. The most preferred adsorbent material is PDMS. In a further aspect the adsorbent article is a fiber or a stir bar coated with an above adsorbent material. The preferred adsorbent article is a stir bar coated with PDMS or PDMS without support such as a film made of PDMS.

In a further aspect the analyte is selected from one or more of the following:

- pharmaceutically active compounds,
- cosmetically active compounds,
- toxic compounds,
- pheromones or hormones,
- proteins, carbohydrates or fats present in food,
- flavours,
- compounds inducing a physical perception,

or a degradation product of the above.

Preferably, flavours are selected from compounds inducing a chemoreception and compounds inducing a trigeminal perception. Preferably, compounds inducing a physical perception are selected from compounds inducing a haptic perception, compounds eliciting a sensation selected from temperature, pain, astringency, and mouth feel.

It is also preferred that the analyte is selected from proteins, carbohydrates, fats, tastants or other compounds inducing any kind of chemo- or physio-perception, types
of compounds eliciting a trigeminal sensation in the in the nasal, oral or pharyngeal area, volatiles and odours. Most preferably, the analyte is selected from a volatile, tastant, odorants or a degradation product thereof.

Most preferably the analyte is an odorant.

In a further aspect desorption is made by thermal desorption.

In a further aspect detection is performed by GC, preferably by GC/MS, GC/Olfactometry or GC/MS/Olfactometry. Most preferred is high resolution gas chromatography (HRGC/O).

The period of extracting the analyte from the defined area of the body ranges from 1 min to 24 h, preferably from 1 min to 1 h.

If extraction takes places in the oral cavity the period of extracting is preferably from 1-10 min, more preferably from 2-5 min, more preferably from 4-5 minutes and preferred 5 min.

If extraction takes places at the skin the period of extracting is preferably from 1 min to 5 h, more preferably from 10 min to 2 h, preferred from 10 min to 1 h, most preferred 30 min.

If a composition comprising the analytes or a precursor thereof is administered prior to extraction the starting point for the application of the adsorbent article and the area of the body ranges from 15 sec to 2 days after administration of the composition.

If extraction takes place in the oral cavity the starting point for the application of the adsorbent article preferably ranges from 15 sec to 25 min, preferably from 1 min to 20 min, preferred from 1 min to 5 min, after elimination of the composition from the mouth.
If extraction takes place at the skin the starting point for the application of the adsorbent article preferably ranges from 2 min to 48 h, preferably from 1 h to 12 h after administration of the composition.

In an embodiment the method comprises the following steps:
   a) oral administration of a composition comprising the odorants or precursors thereof, where the composition is selected from food, a matrix spiked with odorants or a beverage, or tobacco-ware to a subject
   b) contacting an adsorbent with the saliva from said subject at predefined starting point, where the adsorbent material preferably is PDMS
   c) extracting the analyte for defined period from said saliva
   d) thermal desorption of the analyte from the adsorbing material
   e) detection of the analyte by GC/MS, GC/Olfactometry, GC/MS/Olfactometry. Most preferred is high resolution gas chromatography (HRGC/O)
   f) steps a-e) carried out more than once where the starting points in b) differ from at least 15 sec and the extraction period in c) does not vary.

In a further embodiment the method comprises the following steps:
   a) oral administration of a composition comprising the odorants or precursors thereof, where the composition is selected from food, a matrix spiked with odorants or a beverage, a mouthwash or tobacco-ware to a subject
   b) contacting an adsorbent with the saliva from said subject at predefined starting point, point selected from 15 sec to 5 min, preferred from 15 sec to 2 min after elimination of the composition from the mouth where the adsorbent article is a stir bar coated with PDMS or a film made of PDMS.
   c) extracting the analyte from said saliva
   d) thermal desorption of the analyte from the adsorbing material
   e) detection of the analyte by GC/MS, GC/Olfactometry or GC/MS/Olfactometry. Most preferred is high resolution gas chromatography (HRGC/O)
   f) steps a-e) carried out more than once where the starting points in b) differ from at least 15 sec and the extraction period in c) does not vary.

In one embodiment the method comprises the following steps:
a) oral administration of a composition comprising the odorants or precursors thereof, where the composition is selected from food, a matrix spiked with odorants, a beverage, a tobacco-ware or toothpaste to a subject

b) introducing an adsorbent into the mouth of said subject at predefined starting point, where the adsorbent material preferably is PDMS
c) extracting the analyte for defined period from the saliva, removing the adsorbent article from the mouth
d) thermal desorption of the analyte from the adsorbing material
e) detection of the analyte by GC/MS, GC/Olfactometry, GC/MS/Olfactometry, Most preferred is high resolution gas chromatography (HRGC/O)
f) steps a-e) carried out more than once where the starting points in b) differ from at least 15 sec and the extraction period in c) does not vary.

A further embodiment comprises the previous method where the starting point is selected from 15 sec - 5 min, preferred from 15 sec - to 2 min after elimination of the composition from the mouth.

A further embodiment comprises the previous methods where the adsorbent article is kept for 5 min within the mouth.

In a further embodiment the method comprises the following steps:
a) oral administration of a composition comprising the odorants or precursors thereof, where the composition is selected from food, a matrix spiked with odorants, or a beverage, a mouthwash, or tobacco-ware to a subject

b) introducing an adsorbent article, preferably a stir bar coated with PDMS, or film made of PDMS, into the mouth of said subject at predefined starting points selected from 15 sec-15 min, preferably from 15 sec to 5 min, and more preferred from 15 sec to 2 min, after elimination of said composition
c) extracting the analyte for 5 min from said saliva in the mouth
d) thermal desorption of the analyte from the adsorbing material
e) detection of the analyte by HRGC/O.
f) steps a-e) carried out more than once where the starting points in b) differ from at least 15 sec and the extraction period in c) does not vary.

In a further embodiment the method comprises the following steps:

a) topical administration of a composition comprising the odorants or precursors thereof, where the composition is selected from a medicament or cosmetic, perfume, skin care, hair-wash, deodorant, ointment, cream, sun cream, lotion, soap, shampoo, or other rinsing product.

b) applying an adsorbent onto the skin of said subject at predefined starting point, where the adsorbent material preferably is PDMS

c) extracting the analyte for defined period from the skin or the headspace of that area, removing the adsorbent article from the skin

d) thermal desorption of the analyte from the adsorbing material

e) detection of the analyte by GC/MS, GC/Olfactometry, GC/MS/Olfactometry, Most preferred is high resolution gas chromatography (HRGC/O)

f) steps a-e) carried out more than once where the starting points in b) differ from at least 5 min and the extraction period in c) does not vary.

A further embodiment comprises the previous method where the starting point is selected from 1h to 12 h after application of the composition to the skin.

A further embodiment relates to the methods as mentioned above where the defined area of the skin are the armpits.

The present invention also provides an adsorbent article suitable to be applied in the above method comprising:

- a housing having at least three of apertures located in a manner that they allow a free flow of a fluid into and out of the housing,

an adsorbent material included within this housing.

Preferably, the adsorbent article comprises a porous capsule and an adsorbent material included therein. In an embodiment, the housing is made of metal, glass,
silicone, plastic, ceramics or porcelain. Preferably, the capsule is made of glass and is suitable to be introduced into the mouth.

In one embodiment, no further liquid-absorbing material is added to the adsorbent material. Preferably, the weight increase of the adsorbent material when exposed to a liquid is 0 to 5 weight % (20°C, 10 min).

In an aspect of the present invention, the adsorbent material allows a thermal desorption of an analyte from same. Preferably, the adsorbent material allows an adsorption of an analyte by means of physiosorption.

It is preferred that the housing has the form of a tube which has apertures distributed over the tube. More preferably, the tube is releasably closed at both ends. In another embodiment, the housing has at least one flat surface with apertures distributed over said surface. In one embodiment, the housing is disposable.

The invention further relates to an adsorbent article included in a porous capsule. The capsule may be made of glass and suitable to be introduced into the mouth. In a preferred embodiment the adsorbent material is made from PDMS. In a embodiment the absorbent article is a stir bar, preferably coated with PDMS. In another embodiment the adsorbent article is a film made of PDMS. Preferably the capsule measures 15 mm or 25 mm in length.

The present invention further relates to a patch comprising a layer of an adsorbent material and a support provided on said adsorbent material. The patch is designed in a manner that the adsorbent material such as a film of can be applied to the skin. Preferably, the support comprises a backing layer having provided thereon a layer of an adhesive. The layer of an adhesive might be present as discontinuous or as continuous layer. The adsorbent material can be easily removed from the patch. The adsorbent material might be attached to the backing layer via the adhesive layer. In case the absorbent material is fixed to the patch, only a small part of it should be fixed, but not with more than 40 % of the surface of the absorbent article. According
to one embodiment, 5 to 40% of the surface of the adsorbent material is attached to
the backing layer.
Preferably the adsorbent material is not fixed to the patch.
The adsorbent material preferably is PDMS.

The present invention also relates to the use of an adsorbent article for determining
qualitatively or quantitatively one or more analytes. Preferably, the use is in solid
phase extraction. Preferably, the use is in the above method.

The present invention further relates to the use of a patch for determining
qualitatively or quantitatively one or more analytes. Preferably, the use is in the
above method.

The present invention is further directed to the use of the above method for selecting
relevant compounds for the manufacture of a composition to be administered to a
subject. The invention is directed in on aspect to the use of compounds which have
been determined to be relevant according to the above method for the manufacture
of a composition to be administered to a subject.

The invention further relates to a method for determining qualitatively or quantitatively
one or more analytes present at the surface of the skin after topical administration of
a composition to a subject characterised by the following steps:
a) topical administration of a composition comprising the analytes or a precursor
thereof to defined area of the skin of a subject
b) contacting an adsorbent article with the defined area of the skin from said subject
at predefined starting point, where the adsorbent article preferably is a stir bar
coated with adsorbent material, such PDMS, or a film made of PDMS
c) extracting the analyte for defined period from area of the skin
d) desorption of the analyte from the adsorbing material
e) detection of the analyte
f) optionally steps a-e) or b-e) are carried out more than once where the starting
point in b) differs and optionally the extraction period in c) may vary.
The invention further relates to said method where the defined area of the skin is the area under the armpits.

The invention further relates to said method where the defined starting point is from 0 sec to 48 h, preferably from 1 min to 24 h, and more preferred from 5 min to 12 h.

Definitions / Explanations

To facilitate an understanding of the present invention, a number of terms and phrases are defined and explained below. Also embodiments for specific terms are included

Subject
The term "subject" means human being or animal. The term includes men and women, independently from their age.

Method
The method in accordance with the present invention is non-invasive, which means that it does not include a surgical treatment. Specifically, there is no physical impact on the defined area of the body.

Adsorbent article
As used herein the term "adsorbent article" means an article comprising an adsorbent.

The term "adsorbent " as used herein means an area where a substance to be assayed is immobilised.

As used herein, the term "immobilisation" refers to attachment or entrapment, either chemically or otherwise, of material to another entity (e.g. a solid support, substrate, or surface) in a manner that restricts the movement of the material.

The adsorbent material must be suitable to adsorb the analyte.
The term adsorbent article includes articles which only consists of adsorbent material (such foils, sheets, films or fibers made of the adsorbent material) or comprises a support.

In the latter case the adsorbent material may be incorporated, enclosed or coated to a support.

The term support means any material that provides solid or semisolid structure with which another material can be incorporated, enclosed or coated. Such materials include smooth supports (e.g. metal, glass, plastic, silicon, ceramics) as well as textured and porous materials.

Such materials also include, but are not limited to, gels, rubbers, polymers, and other non rigid materials.

Preferred adsorbent articles are fibers or stir bars as commonly used in solid-phase microextraction (SPME) or stir bar sorptive extraction (SBSE).

For some needs a film made of PDMS may be preferred.

Preferably the adsorbent material is selected from the above materials, more preferably polydiakylsiloxanes such as polydimethylsiloxane (PDMS), divinylbenzene, carbowax /divinylbenzene, carboxen/PDMS, PDMS/divinylbenzene, carboxen/divinylbenzene, polyacrylate. The preferred adsorbent material is PDMS.

The preferred adsorbent article is a stir bar, comprising a first and innermost part which is a magnetic rod, a second part which is a thin glass jacket covering the magnetic stirring rod and a third outermost part which is a adsorbent layer of PDMS.

Such an article is commercially available from Gerstel GmbH, Germany called Twister®.

For use in the oral cavity the material used must be physiologically acceptable and must not be toxic, as proved for PDMS within the present invention.

The size and shape of the adsorptive article as well as surface area or coating thickness of the adsorptive layer may adapted to the needs.
The adsorptive article may be described by a thickness A, mm, a width B mm, and a
length C mm. Preferably the A, B, C have a value of below 30 mm, preferably 20 mm
or below and preferred 10 mm or below.

In one embodiment a stir bar is used having a length C below 30 mm, preferably 20
mm or below and preferred 10 mm or below.

In one embodiment, the adsorbent article may be described by a diameter A and a
length B. For introduction into the mouth the parameters A and B preferably have a
value of below 30 mm, preferably 20 mm or below and preferred 10 mm or below.

For application to the skin the parameters A and B might have different values.
In the preferred case a stir bar is used having a length B below 30 mm, preferably 20
mm or below and preferred 10 mm or below and having a diameter A below 5 mm.

Preferably the adsorptive article has no specific receiving zone for detection of a
particular analyte. Moreover the adsorptive article preferably has no detection zone
for determining the presence of a specific analyte.
Specific receiving zone means e.g. an antibody to a particular analyte.
Detection zone means a reaction site that gives a signal when a specific analyte is
present, such as a biosensor, enzyme reaction system, or antibody.

In one preferred embodiment the adsorbent material is included in a housing having
a plurality of apertures.
The apertures are located in a manner that they allow a free flow of a fluid such as
water into and out of the housing.
Preferably the size of apertures is such that the adsorbing material is prevented from
leaving the apertures and permitting the fluid to be analysed to flow freely into and
out of the housing.
Preferably the size of the holes ranges from 0.05-5 mm, preferably from 0.1-2 mm
and more preferred from 1-1.5 mm.
The housing is made of a chemically inert material, such as ceramic (transition metal
oxides), metal, porcelain or glass. Preferred are porcelain or glass. Most preferred is
glass. When the housing is made of plastic, it can be selected from PET (polyethylene terephthalate), PETG (polyethylene terephthalate, glycol modified), PBT (polybutylene terephthalate), PC (polycarbonate), PVC (polyvinylchloride), PP (polypropylene), PE (polyethylene, including low density and high density PE), PS (polystyrene), PEN (polyethylene naphtalate), COC (cyclic olefin copolymer), POM (Polyoxymethylene), EVOH (Ethylene Vinyl Alcohol), PAN (Polyacrylonitrile), PA (polyamide such as nylon), LCP (liquid crystal polymer), TPE-E (Thermoplastic Copolyesters). Apart from the above-mentioned apertures, the plastic material preferably has no pores but has a smooth surface.

The shape and the size of the housing is adapted to the place where the analyses should take place.

Thickness A, a width B and a length C of the housing, e.g. capsule, have preferably a value 5 mm higher than those from the adsorbent article.

The housing may have the shape of a tube, where one or both ending could be removable. The tube may have a length from 0.5 cm - 5 cm, preferably from 1-2 cm. It might have a width/diameter from 0.2 cm to 2 cm, preferably 1 cm.

The housing may have one flat side, e.g. the housing might have the shape of tube which is cut in the middle. One or both endings of the "half-tube" might be closed with a removable lid. The housing may have a length from 0.5 cm - 5 cm, preferably from 1-2 cm. It might have a diameter from 0.2 cm to 2 cm.

The tube having a diameter from 0.5 cm -1 cm and having a length from 1-2 cm for example is suitable for analysing compounds in body cavities such as the mouth, vaginal or anal cavity, or armpits.

Housings having a flat side are suitable for analysing portions of the skin.

In case the housing has the form of a capsule or closed tube the apertures may be located at their longer site.

The housing may have any other shape suitable for the present invention. Shapes include spherical, cubical, or a random shape which can be adapted, e.g., to the respective area of the body.

No further housing than the housing mentioned above is arranged around the adsorbent article when used in the above method.
The adsorbing material included within the housing material may have the form of a powder, fibers, beads, glass beads coated or linked with the adsorbent material, capsules, micro-capsules, pellets micro-pellets, or a sheet, film or foil of the adsorbing material. The adsorbent material might be plain, porous or hollow. The sheet, film or foil might be folded.

The adsorbent material is adapted to the housing, e.g. beads of adsorbent material such as PDMS or Tenax might have a diameter from more than 0.05 mm to below 10 mm. Preferred are beads, comprising PDMS (consisting of PDMS or coated with PDMS), having a diameter from more than 0.05 mm to below 10 mm, preferably from more than 0.5 mm to below 5 mm and most preferred from more than 1 mm to 2 mm.

A magnetic stirrer may be placed additionally within said housing.

The magnetic stirrer might be coated with the adsorbing material. In this case no additional adsorbing material has to be present, but might be.

The adsorbent material is chemically inert, and does not release any compounds. The adsorbent material preferably is capable to adsorb odorants or tastants. All materials as mentioned above are suitable. Preferred materials are PDMS and Tenax®.

Preferably, the adsorbent material is removable from the housing. The term "removable" means in this context that the adsorbent material is not physically attached to the housing. Preferably, the adsorbent material is free flowing within the housing.

In one embodiment, the adsorbent article comprises a means for ensuring the safety of the subject, particularly when an oral application is contemplated. Such a means can be a fixing, holding and/or retrieving means. Particular examples of such a means include a string, thread, wire or hook.

In one embodiment the adsorbent material may be introduced into capsule. The term apertures means that the capsule is porous to allow an unhindered penetration of air and saliva to the adsorbent article. The capsule preferably is made from glass and
closed with a cap. Thickness A, a width B, and a length C of the capsule have preferably a value 5 mm higher than those from the adsorbent article. The pore size may vary from 0.5-5 mm, preferred from 1-2 mm.

The parameters, such as surface of the adsorbing material, period of contact, size of the adsorbing article may be varied according to the needs. For instance the surface of the adsorbing material may chosen in a way, that the absorption is in relation to the threshold of detection. Thus it might be possible to adjust the parameters in a manner that analytes are only detected if they are present in a concentration above the nasal threshold.

Experiments have shown that an increase of the surface e.g. by use of a folded sheet or beads (in comparison to a coated magnetic stirrer or a fiber) the amount of analyte adsorbed can be increased, or, the contact time can be decreased without significantly prolonging desorption time. This is an important aspect, if differences between short intervals are to be detected, and/or the contact time should be rather short. On the other hand even small amounts of the analyte could be detected.

Composition

The term oral composition (to be administered prior to the extraction of the analytes) means any kind of food (liquid or solid) (including regular meals, sweets, chewing gum, nutritional supplements), beverages (such as fruit juice, mineral drinks, lemonade, infusions, alcoholic drinks including wine and beer, caffeine drinks such as coffee, espresso, cappuccino, black or green tea, energy drinks), matrixes enriched with compounds to be analysed, pharmaceutical compositions, mouthwashes, toothpaste, tobacco-ware especially smoke thereof (i.e. smoke from cigarettes, pipes, cigars) or perfumes.

The term topical composition (to be administered prior to the extraction of the analytes) comprises ointments pastes, lotions, creams, gels, sun creams, perfumes, shampoos, soaps, skin care, showering gels, body rinsing materials, TTS (transdermal therapeutic systems). Topical compositions may be used cosmetically or therapeutically.

Analyte

The term analyte means any compound that may be analysed.
The term relates to any compound to be administered orally or topically or to the nasal vaginal or anal cavity. The analyte may be ionic or non-ionic, polar, non-polar or semipolar. The term analyte includes pharmaceutical actives, cosmetic actives, adjuvants, hormones, pheromones, proteins, toxic compounds (e.g. environmental toxics), carbohydrates, fats, tastants or other compounds inducing any kind of chemos- or physio-perception, types of compounds that elicit a trigeminal sensation either in the nasal, oral, or pharyngeal area, volatiles, or odours. Preferred analytes are tastants, volatiles, and odorants. Most preferred are odorants.

Tastants are defined as compounds interacting with taste receptors located in taste buds of the tongue. Five important basic taste perceptions exist: sour, sweet, bitter, salty and umami.

Chemo-reception or physio-perception e.g. means compounds that elicit sensations of heat, coolness, astringency, spicy, burning or hot sensations, pungent soapy or fizzy sensations, perceptions of creaminess or other types of mouth feeling. Odorants (or other expressions are odours, flavours or aroma substances) are volatile compounds which are perceived by the odour receptor sites of the smell organ i.e. the olfactory tissue of the nasal cavity.

The aforementioned odorants may be largely classified into aldehydes, esters, acids, ketones, aromatic compounds, ethers, and epoxides. A list of odorants to be used can be found in the attachment.

The term odorant comprises naturally occurring odorants, precursors thereof, or synthetically prepared odorants or precursors thereof.

The term "analyte" also includes degradation products or metabolites of compounds included within the composition to be administered orally. This may be especially relevant for compounds that are already metabolised within the oral cavity. Preferably, the term analyte includes compounds that degrade to odorants or degradation products of odorants. The term also relates to odorants which are formed within the oral cavity.

In addition, compounds which are metabolised after swallowing are included. Preferred are metabolites which are odorants.
Administration

The term oral administration means:
putting a composition into the mouth or inhalation of a composition, where the compositions optionally is kept in the oral cavity, rinsed or masticated in the mouth or kept in the respiratory tract (for inhalation) for a determined period of time and finally swallowed, spit out or exhaled.

Topical administration means:
Applying a composition to the skin and optional washing of the area.

Contacting an adsorbent article with saliva

Contacting an adsorbent article with saliva means introducing the adsorbent article into the mouth.

Starting point

Starting point means a defined moment after administration of a composition to the body.

Starting point after oral administration of a composition defines a moment where the adsorbent article is put into the mouth after administration of a composition into the mouth or after inhalation of a composition. The starting point may be a moment where the composition is still in the mouth.
In a preferred embodiment it defines a moment after elimination of the composition from the mouth, such as a defined moment after swallowing, spitting out, or exhalation of the composition.
The starting point can be any moment between 0 sec and 48 h after putting a composition into the mouth or after elimination of the composition of the mouth.
Preferably the starting point is selected from 15 sec to 2h, more preferably from 15 sec to 25 min after elimination.
In the case that the method is carried out several times, the starting points may vary.
In one embodiment the starting point of the first determination will be 15 sec, the starting point of the second determination will be 30 sec, the starting point of the third determination will be 60 sec. Variation thereof will be a matter of routine for the skilled worker.
In case the composition is administered topically, or to the vaginal, anal or nasal cavity the starting defined the moment where the adsorbent article is applied to the defined area after administration of the composition or after removal such as washing of the composition. If not otherwise stated herein it defines the interval after administration of the composition.

**Extraction period**
The period of extracting the analyte from the defined area of the body ranges from 1 min to 24 h, preferably from 1 min to 1 h.

If extraction takes place in the oral cavity the period of extracting is preferably from 1-10 min, more preferably from 2-5 min, more preferably from 4-5 minutes and preferred 5 min.

If extraction takes place at the skin, the period of extracting is preferably from 1 min to 5 h, more preferably from 10 min to 2 h, preferred from 10 min to 1 h, most preferred 30 min.

Since application of the adsorbent article for a longer period such as 30 min, may cause changes of the conditions at the skin (e.g. changes in permeation behaviour, swelling), in some cases it may be advantageous to select an extraction period of less than 10 min.

**Extraction period from saliva**
Extraction period from saliva means a defined period in which the adsorbent article stays in contact with the saliva.

This simply means keeping the article within the mouth, where preferably the mouth is closed.

According to the needs, it may be preferred to keep the adsorbent article within a defined area of the mouth, e.g. sublingually, on the tongue in the cheek, etc.

In some cases it may be preferred not come into touch with some areas of the oral cavity, e.g. oral mucosa. Accordingly, the use of an adsorbent article which is protected from contact with the oral tissue, i.e. by a capsule (see adsorbent article) may be advantageous.
The extraction time may be selected from 1-10 min, more preferably from 2-5 min, more preferably from 4-5 minutes and preferred 5 min.

*Desorption*
Desorption means release of the analytes from the adsorbent article. Desorption is mainly dependant form the chemical and physical properties of the analyte.
The selection of the appropriate method of desorption is a matter of routine for the skilled worker. After extraction the adsorbent article may optionally shortly rinsed with purified water and dipped on a clean paper tissue to remove water droplets prior to desorption.
Desorption can be carried out by liquid desorption. A preferred solvent may be acetonitril, methanol, ethanol, or ethylacetat, Ethers such as diethylether, or dichloromethan. Appropriates techniques such as the use of ultrasound are known in the art.
Desorption also can also be carried via thermal desorption. Desorption temperatures are primarily dependent by the volatility of the analyte and is typically between 150-300 °C.

Thermal Desorption can be accomplished by flow of a carrier gas such as helium. Thermal Desorption may be combined with cold trapping and reconcentration (cryofocusing).

*Detection*
Detection means detecting the presence of the analytes and optionally quantifying. The following methods are illustrative examples not limiting the invention in any way.

Samples may be analyses by HPLC or LC. For detection, mass spectroscopy (MS) or UV may be used.
The sample may be derivatised. This method is especially relevant for liquid desorption.
Volatile analytes preferably are analysed by GC. For detection MS, FID, chemosensors, artificial noses, Olfactometry or combinations thereof, such as FID/Olfactometry MS/Olfactometry may be used. Preferred is detection by high-resolution gas chromatography-olfactometry (HRGC/O). Olfactory is the determination of compounds by nasal receptors.

In order to detect odorants the retronasal threshold advantageously is taken into account.

The present studies have shown that the retronasal threshold may be correlated to the GC/Olfactometry detection, meaning that mainly concentrations are detected that are relevant for retronasal perception. Sensitivity of GC/Olfactory detection may be influenced by gas flow through the GC, desorption time, sniffing port temperature, oven temperature program, material of the stationary phase.

In addition, adsorption to the adsorbent article may be varied in order to obtain correlation between retronasal relevance and detection.

In another embodiment the adsorbent article prior to desorption may be introduced into a sample comprising standards prior to desorption. Preferably, those standards are isotope labelled analytes.

These analytes may be present in an amount relevant for retronasal perception.

**Detailed description**

The following description highlights several preferred embodiments of the present invention. The present invention is not limited to these illustrative examples. While the following description highlights the use within the oral cavity, it should be understood that extraction in vitro are within the scope of the present invention.

**Figures**

Figure 1. Perforated glass capsules for intraoral application of SBSE bars in BOSS-analysis.
Figure 2. Initial retronasal intensity during oral application of the single odorant solutions versus retronasally perceived persistence of the same odorants.

Figure 3. Time-resolved intraoral odorant detection by BOSS after expectoration of single odorant solutions versus the respective retronasal sensory persistence.

Figure 4. Time-resolved retronasal evaluation of the intensities of odor attributes and their overall odor intensities (middle graph) after intraoral application and expectoration of strawberry aroma samples in water and milk, respectively.

Figure 5. Retronasal sensory persistence of odor attributes after intraoral application and expectoration of strawberry aroma samples in water and milk, respectively.

Figure 6. Comparison between time-resolved (15, 30, 60, 120, 240 sec) intraoral odorant detection by BOSS after expectoration of aqueous strawberry aroma sample (left) and the respective retronasal odor activity values in water (ROAV, right).

Figure 7. Time-resolved (15, 30, 60, 120, 240 sec) intraoral odorant detection by BOSS after expectoration of strawberry aroma samples in water and milk, respectively.

Figure 8. Time-resolved retronasal evaluation of the intensities of odor attributes and their overall odor intensities (middle graph) after intraoral application and expectoration of two Chardonnay wines.

Figure 9. Comparative BOSS of two Chardonnay wines.

Figure 10a. Housing including an adsorptive material suitable to be introduced into the mouth, vagina, anal cavity, nose, under the armpits or for solid phase extraction.
A: adsorbent material; B: Housing (tube); C: apertures; D: releasable closing

Figure 10b. housing including an adsorptive material suitable to be introduced into the mouth, vagina, anal cavity, nose, under the armpits or for solid phase extraction.
A: adsorbent material; B: Housing (capsule); C: apertures;

Figure 10c: housing including an adsorptive material suitable to be applied onto the skin
A: adsorbent material; B: Housing (tube cut in the middle); C: apertures; D: releasable closing

Figure 10d: housing including an adsorptive material suitable to be applied onto the skin
A: adsorbent material; B: Housing (watch glass); C: apertures

Figure 10d: patch including an adsorptive material suitable to be applied onto the skin
A: adsorbent material; E: adhesive layer; F: backing layer; G: optional fixing means for the adsorbent material to the backing layer

MATERIALS AND METHODS

Chemicals
The following odorants were obtained from the suppliers shown: ethyl butanoate, ethyl 2-methylpropanoate, ethyl 3-methylbutanoate, ethyl hexanoate, butane-2,3-dione, pentan-2,3-dione, 2-furfurylthiol, hexanal, (Z)-3-hexenol, 2,5-dimethyl-4-hydroxy-3(2H)-furanone, 3-isobutyl-2-methoxy pyrazine, 2-ethyl-3,5-dimethylpyrazine, 3-(methylthio)-propanal, 3-methylbutanal, 2/3-methylbutanoic acid, (E,E)-2,4-nonadienal, (E)-2-nonenal, octanal, γ-decalactone (Aldrich, Steinheim, Germany), acetic acid, butanoic acid, 2-methoxyphenol, vanillin (Merck, Darmstadt, Germany), (E)-β-Damascenone (Haarmann and Reimer, Holzminden, Germany), β-ionone (Roth, Karlsruhe, Germany), (E/Z)-2,6-nonenadienal (Alfa Products, Karlsruhe, Germany), 1-octen-3-one, 4-vinyl-2-methoxyphenol, (Z)-3-hexenyl acetate
(Lancaster, Mühlheim, Germany), methyl cinnamate, styrrlayl acetate, benzyl acetate, methyl dihydrojasmonate (Givaudan, Dübendorf, Switzerland), methyl anthranilate (Merck, Darmstadt, Germany). trans-4,5-Epoxy-(E)-2-decenal was synthesized according to (18). The compounds were freshly distilled prior to analysis. Chemical and sensory purity was checked by gaschromatography-olfactometry (GC/O) as well as gaschromatography-mass spectrometry (GC-MS).

**Strawberry Aroma**

The strawberry aroma was obtained from Givaudan (Dübendorf, Switzerland). The composition of the aroma is given in Table 1.

**Chardonnay Wines**

The following chardonnay wines were selected for investigation: 1999 Merryvale Reserve Chardonnay, 14.5 % by vol., Napa Valley, Merryvale Vineyards (St. Helena, California, USA) and 2002 Forest Hill Chardonnay, 13.5 % by vol., Jindalee Estate P/L (Moorabool, Victoria, Australia).

**PDMS-coated stir bars**

For the experiments, commercially available Twister®-SBSE bars (Gerstel GmbH, Mühlheim a/d Ruhr, Germany) in the sizes given in Table 2 were used. Prior to analysis, the bars were subjected to a condition procedure according to the suppliers recommendations: the stir bars were first soaked in 100 % acetonitril for at least two days, then conditioned at 300 °C for 4h. Prior to analysis, each SBSE bar was first screened for odorants ("background", see "Results and Discussion") and then directly applied for analysis. Each stir bar was used for just one single experiment, then reconditioned and screened for background again. Each experiment was performed with at least three different SBSE bars to avoid SBSE bar variation.

**Encapsulation of the SBSE bars**

For intra-oral application, adapted glass capsules were designed (cf. Figure 1). For the 20 mm bars, the total length of the capsule was 25 mm, for the 10 mm bar 15 mm. The inner diameter was in both cases 5 mm. The capsules were sealed with a glass stopper. To allow unhindered penetration of air and saliva, the capsules were regularly perforated with pores (1-2 mm diameter) with a distance of about 3 mm between pores.
Preparation of the aqueous odorant model solutions

1.0 % stock solutions of the single odorants in absolute ethanol were freshly prepared and diluted with deodorized water prior to analysis to obtain 500 mL of single aqueous solutions of each odorant (concentration: 100 µg/L and 1000 µg/L water, respectively). From these, the respective concentrations of the odorants at their retronasal odor threshold values (ROTV), at 10-fold lower concentrations (0.1 ROTV) or at the concentrations given in Table 1 were prepared by further dilution with deodorized water.

Preparation of Strawberry Aroma Samples

The aroma stock solution was diluted with pure EtOH. From this aroma solution 100 µL were pipetted into 100 mL of water or milk (3.5 % fat, UHT) to obtain the final odorant concentrations as given in Table 1.

Sample Preparation

1 mL of each aqueous aroma solution was pipetted separately into 10 mL closed glass vessels. The stir bar was immediately placed in the respective sample, stirred for 5 min, removed with tweezers, dipped into deodorized water, briefly dried with lint-free tissue and immediately placed into the thermodesorption unit.

Intra-oral Sampling of Odorants

Panelists were non-pregnant volunteers (non-smokers) of the Technical University of Munich, exhibiting no known illnesses at the time of examination and with normal olfactory and gustatory function. Subjective aroma perception was normal in the past and at the time of examination. The panelists had a normal salivary flow and were selected for their excellent oral hygiene, thereby not suffering from oral diseases and nuisances, such as plaque, caries, tartar, gingivitis and periodontitis. Intra-oral analyses were performed 2 hrs after breakfast and thorough cleaning of the teeth and oral cavity with a commercial toothpaste (5 min) and with a commercial alcohol-free, low-aromatized and antimicrobial mouthwash. Prior to oral application of the sample, the oral cavities of the panelists were screened for odorants ("blank", see Discussion chapter).

Then, 25 mL of the respective sample were taken into the oral cavity, kept for 10 sec with closed lips and closed velum and rinsed carefully within the oral cavity, then expectorated. At defined time intervals (2-fold increase) after expectoration (15 sec, 30 sec, 60 sec, etc.), an extraction capsule containing one SBSE bar was placed in
the oral cavity. The lips and velum were kept closed and the capsule was moved carefully within the oral cavity, thereby avoiding swallowing actions. After 5 min of equilibration, the capsule was removed from the oral cavity; the SBSE bar was removed with tweezers, dipped into deodorized water, briefly dried with lint-free tissue and immediately placed into the thermodesorption unit.

**SBSE Thermodesorptive Sample Application**

Thermodesorption of the samples was performed by means of a TDS-2 thermodesorption system (Gerstel GmbH) in combination with a CIS-4 PTV injector (Gerstel GmbH) for cryofocusing the analytes prior to transfer onto the analytical column. The following sampling parameters were used:

Splitless thermal desorption was performed by programming the TDS-2 from 40 °C to 240 °C (5 min) with a rate of 60 °C. Cryofocussing was performed with liquid nitrogen at −100 °C. Injection was performed with a ramp of 12 °C/s from −100 °C to 240 °C (5 min). The gas chromatographic conditions are given below.

**Rating of Odorants using the BOS-System**

Detectability of the odorants was based on their sensory properties, that means first and foremost on their odor intensities. That means that only those substances were rated as detectable by the Buccal Odor Screening System (BOSS) which were perceived by HRGC/O. Detection by HRGC/MS or HRGC/FID was not taken into account as this does not necessarily correlate with the sensory impact of the respective compound.

**High Resolution Gas Chromatography-Olfactometry**

Application of the samples was either performed as described above (*SBSE Thermodesorptive Sample Application*) or by the cool on-column injection technique at 35 °C (solvent extract samples). The odorants were screened in parallels by five panelists by sniffing the effluent either after one-or two-dimensional gas chromatography. Sniffing analysis was repeated five times by each panelist. All detected odorants were identified by comparison with reference substances on the basis of the following criteria: retention index (RI) on three stationary phases of different polarity (FFAP, SE-54; OV-1701), mass spectra obtained by MS (EI) and MS (CI), and odor quality as well as odor intensity perceived at the sniffing-port. The one- or a two-dimensional gas chromatography system (TD-HRGC) consisted of a Mega 2 gas chromatograph (Fisons Instruments, Mainz-Kastel, Germany) as the
precolumn system in tandem with a Fisons GC 5160 as the main column system. The following fused silica columns were used: DB-FFAP (30 m x 0.32 mm i.d., 0.25 μm FD, J & W Scientific, Folsom, USA) and/or DB-5 (SE-54; 30 m x 0.32 mm i.d., 0.25 μm FD, J & W Scientific, Folsom, USA). The gas chromatographic conditions were the same as described previously (19).

**High Resolution Gas Chromatography-Mass Spectrometry**

The odorants were analysed by two-dimensional gas chromatography (TD-HRGC) as described above. MS analyses were performed with an ITD-800 (Fisons Instruments, Mainz-Kastel, Germany) running in the CI-mode with methanol as the reagent gas. The following fused silica columns were used: DB-FFAP (30 m x 0.32 mm i.d., 0.25 μm FD, J & W Scientific, Folsom, USA) in combination with DB-5 (SE-54; 30 m x 0.32 mm i.d., 0.25 μm FD, J & W Scientific, Folsom, USA). The gas chromatographic and mass spectrometric conditions were the same as described previously (19).

**Isolation of the Wine Volatiles**

100 mL of the respective wine from a freshly opened bottle were extracted with dichloromethane (3 times, 100 mL of solvent and 30 min of extraction time each, total volume of solvent: 300 mL). The combined extracts were dried over Na₂SO₄ overnight, followed by distillation in vacuo (19). For analysis by HRGC/O, the sample was concentrated to a total volume of 10 mL.

**Identification of Odorants**

The odorants were identified by comparing them with the respective reference compounds on the basis of the following criteria: odor quality, odor intensity, retention indices on two capillaries of different polarity (FFAP, SE-54), as well as mass spectra obtained by MS(EI) and MS(Cl).

**High Resolution Gas Chromatography/Olfactometry**

HRGC/O was at least performed three times by three different panelists at different days.

**Quantitation by SIDA**

Quantitation using the respective stable isotope labelled standards was performed as described previously (20). The mass traces for the labelled and the unlabeled compounds are given in Table 7.
Sensory Evaluation

Ten assessors (five male, five female) were recruited from the Technical University of Munich. In preceding weekly training sessions, the panelists were trained in recognising orthonasally and retronasally about 150 selected odorants at different odorant concentrations according to their odor qualities. Participation in these sessions was at least for one year prior to participation in the actual sensory experiments. Panelists were always asked to score odor intensities from 0.0 (not perceivable) to 3.0 (very intense). Sensory analyses were performed in a sensory panel room at 21±1 °C at three different sessions.

Samples were freshly prepared, stirred for 30 min and immediately applied to sensory evaluation. The model mixtures containing the single compounds, strawberry samples or chardonnay wines (25 mL each), were singly presented to the sensory panel for retronasal evaluation in covered glass vessels (capacity 45 mL). The total amount of the sample was taken into the oral cavity, kept for 10 sec with closed lips and closed velum and rinsed carefully within the oral cavity, then expectorated. At defined time intervals (2-fold increase) after expectoration (30 sec, 60 sec, etc.), the intensity of the overall retronasal aroma perception as well as of single predefined odor qualities was rated by the panelists by deliberately opening the velum-tongue border exactly at these times. The results obtained in three different sessions were averaged and plotted in spider web diagrams. The values obtained in different sessions and for the different assessors differed by not more than 10 %.

For comparative evaluation of the strawberry aroma in water and milk, respectively, the water sample was first evaluated; then, after a 15 min break and rinsing of the oral cavity with tap water, evaluation of the milk sample was performed. Panelists were asked to score predefined odor qualities as well as the overall intensities of the samples at given times as described above. Then, panelists were asked to rate the overall difference between both samples from 0.0 to 3.0.

Determination of Retronasal Odor Threshold Values (ROTV)

The conditions for sensory analysis were the same as described above.

Determination of retronasal odor thresholds in a triangular test according to the "forced choice" approach and statistical treatment of the data was performed according to (21). Panelists were presented 25 mL of the respective samples
together with two blanks each. Retronasal evaluation of the samples was performed either by deliberately opening their velum-tongue-border or by swallowing.

RESULTS AND DISCUSSION

SBSE bar selection
The PDMS-coating parameters of the commercially available SBSE-bars are given in Table 2. At the beginning of the experiments, the smallest bar (A) with the lowest thickness of coating and, consequently, the lowest total amount of PDMS was selected. Preliminary investigations showed that the applied SBSE-Bars are applicable intra-orally without any toxicological harm (22).

Determination of "Background"
After conditioning of the SBSE-bars according to the suppliers recommendations, the bars were screened by HRGC/O for remaining traces of odorants (cf. Table 3). It could be shown that a few odorants were always detectable via HRGC/O at trace concentrations but did not reveal any signal by FI detection due to their very low concentrations. The compounds given in brackets revealed only very weak olfactory detection and were often but not always olfactorially detected in the bars. When performing the sniffing analysis under the same conditions with an empty sample tube but without application of the SBSE bar, no odorants were detectable. Therefore, it was clearly shown that the detection of the mentioned odorants is due to adsorption of traces to the SBSE bars even after conditioning. It is assumed that the detection by HRGC/O is on one hand because the mentioned odorants exhibit very high odor potency (extremely low odor thresholds). On the other hand, these compounds can be regarded as ubiquitous odorants as they represent aroma products from broadly distributed substances such as linol and linoleic acid which can not only be found in a broad diversity of food systems but generally in biological materials such as plants, animals etc. Therefore, "contamination" of the overall environment including air with traces of these potent odorants is very likely and is probably unavoidable. For this reason, the presence and the intensity of these substances in the applied SBSE system was always screened prior to the actual analysis and was set as "background".
**Blank Samples from Oral Cavity**

Screening of the untreated oral cavities of the participants by means of sensory analysis, all panelists reported a faint buccal smell, which was described as a bit tallowy, slightly acidic and as the typical buccal smell of healthy people. It was described as only perceivable when directly sniffing the panelists' mouth and was not attributed to any increased oral smell as it is induced by, for example, halitosis. Screening of the untreated oral cavities of the participants by means of SBSE/HRGC/O revealed a weak detection of eight odor active substances, which were detectable at each sampling day (Table 4). Compounds 1, 2, 3 and 5 were detectable with slightly higher intensities compared to the "background" samples. Therefore, the presence of these compounds in the oral cavity could be proofed.

**Validation of the Extraction Parameters**

*In-Vitro SBSE-Screening according to ROT-Values*

With the feature of saliva acting as an aroma extraction and transport system, odorants should be at least present at their ROTV to elicit retronasal aroma perception upon swallowing. Therefore, the following investigations were based on the assumption that for sufficient sensitivity the SBSE system should be capable of detecting odorants at their retronasal odor threshold level (ROTV). This should be preferably valid under the in-vivo extraction conditions and with the parameters used. To proof the sensitivity of the SBSE extraction system under these conditions, aqueous odorant solutions at ROTV level were prepared. Extraction parameters were then adopted from the in-vivo conditions used (see below), that means extraction was performed for only 5 min in 1 mL of sample. This volume corresponds to the amount of saliva, which was found to be present in the oral cavity at rest (prior to the normal repeated swallowing). In total, 29 odorants from different substance groups were selected for investigation. The diversity of the odorants not only with respect to their odor qualities and odor thresholds, but also to their physicochemical parameters (logP values, molecular weight) can be seen from Table 5. Despite these differences it could be shown, that all compounds were detectable under the given extraction conditions. Furthermore, it was found with only one exception (\(\gamma\)-decalactone), that no detection occurred for all compounds at 10-fold lower concentration (0.1 ROTV). It is clear that this observation cannot be a coincidence, however, the reasons for this
phenomenon are not yet fully clear. It might be possible that the relationships between retronasal aroma thresholds and their detectability via SBSE are correlated via their lipophilicity parameters as the adsorption to SBSE bars was also shown to be strongly related to logP values. In addition, the odor intensity of the compounds represents the basis for detection using the HRGC/O approach, not their detectability by e.g. FID or MS. The logical consequence of this is that indeed some substances are detectable sensorically but do not reveal e.g. any FID signal while on the other hand some compounds are detectable via FID but do not yet elicit any sensory perception. In the last case, detection is not counted as "positive". Moreover, if some compounds would have been detectable at significantly lower concentrations, there might have been a considerable overestimation compared to the other substances. This problem seems not to be relevant. It has to be mentioned that butane-2,3-dione, oct-1-en-3-one and β-damascenone were not evaluated at 0.1 ROTV as these compounds are always detectable by BOSS (see discussion on "background" samples). Therefore, a screening of non-penceence is not achievable. It can be concluded that the "olfactory" approach led to a detection situation which represents favorable screening conditions with regard to the evaluation of odorants and their contribution to retronasal odor detectability.

**Retronasal Sensory Evaluation of Single Odorant Solutions versus BOSS**

In addition to the proof of in-vitro detectability of the odorants at their ROTV using the extraction parameters discussed above, the in-vivo performance of the BOS-System was investigated in comparison to the retronasally perceived persistence of the respective odorants:

**Retronasal Sensory Evaluation**

First, single aroma compounds in aqueous solutions (for concentrations, see Table 1) were evaluated with regard to the initial retronasally perceived intensity when introduced into the mouth. Then, their retronasal sensory persistence was profiled as described in *Sensory Evaluation*, following the "time dilution" (TD) approach. This means that the evaluation was performed at 2-fold increasing time intervals, thereby mimicking a dilution-type approach. The reason for this is that according to preliminary sensory experiments the most significant changes in persistent retronasal aroma profiles occur within the first minutes after swallowing, depending on the food
material applied. On the other hand, the more persistent notes usually do not change significantly in their characters, but just simply "fade" away (23).

In Figure 2, the initially perceived intensities (introduction into the mouth) are plotted against their respective retronasally perceived persistence after swallowing. It becomes evident that the initially perceived intensity does not allow any prediction of the further persistence of the odorant in mouth. For example, (Z)-3-hexenyl acetate, which was perceived with the highest initial intensity (3.0), just persisted for two minutes while 2,5-dimethyl-4-hydroxy-3(2H)-furanone with a comparatively low initial intensity of about 1.25 persisted for 8 min. Now the question arises whether for the short-persistence compounds any type of adaptation occurred to the panelists or whether the compounds were indeed not present any more in the oral cavity.

Therefore, the odorants were screened for their detectability after application to the oral cavity (cf. Intra-oral Sampling of Odorants) using the BOS-System.

The total detection times of both approaches, the analytical using the BOS-system, as well as the sensory by retronasal evaluation of persistence are plotted against each other in Figure 3. The correlations between the results obtained by both techniques are striking. The results strongly emphasize that the short-persistence odorants are indeed not present for longer time in the mouth and that on the other hand the sensory perception is precisely correlated to the presence of odorants in the mouth. In conclusion, it could be clearly shown that BOSS-detection under these conditions (optimized for in-vivo application, see Experimental Section) is directly related to what is perceivable by the panelist/consumer. This in-vivo confirmation of a direct link between odorant concentrations and sensory perception has been achieved in this study for the first time.

**Strawberry Aroma**

**Sensory Evaluation**

In preceding sensory evaluations, the odor qualities citrus, buttery, sweaty, vanilla, grassy, caramel, peach, flowery and fruity were selected. They were either attributed by the panelists as descriptors for the aroma mixture or for the single compounds. Then, the intensities of these odor qualities as well as the overall odor intensities were rated comparatively both in the aromatized water and milk samples at given times (cf. spider web graphs in Figure 4). In parallels, the overall aroma intensities should be rated at the same times (cf. small bar diagrams in Figure 4). When first
looking at the overall aroma intensities and their persistence with time, it becomes evident that the water sample elicits a considerably higher aroma impression than the milk sample from the beginning until the end of evaluation. Regarding the single odor attributes, mainly the flowery, fruity, caramel- and peach-like odor notes were perceivable with significantly higher intensities in the water sample compared to the milk sample at 30 sec (Figure 4a). This effect was not so distinct for the grassy and citrusy impressions, which were generally rated as much less intense than the previous qualities. On the other hand, characteristic milk notes such as buttery and sweaty were more intense in the milk sample. This can be expected as the milk matrix adds certain amounts of aroma compounds such as pentan-2,3-dione and butanoic or methylbutanoic acid to the mixture. However, no quantisation of these compounds was performed in the present study as the focus laid on the changes in the strawberry aroma related odor qualities. When looking at the changes in both aroma profiles with time, it becomes evident that the fruity, flowery, peach- and caramel-like notes persist much longer and with higher intensities in the water sample (up to two and four minutes, respectively). In milk, they were only perceivable for one min and with lower intensities. On the other hand, the buttery and sweaty notes persisted in the milk samples for up to four minutes but were merely undetectable in the water samples, as one would expect. For a better comparison of the total perception, durations of each odor quality see Figure 5. In addition, the persistence with time for the grassy and the citrusy note was higher in the water samples (2 min) than in milk (30 sec and 1 min, respectively). Interestingly, the vanilla note was at first (30 sec) rated as more perceivable in the milk sample but persisted then longer (2 min) in the water sample as compared to the milk sample (1 min). The reasons for this have not been seized at present. It can be assumed that the dominant sweet, flowery and fruity impressions at the beginning of the evaluation lead to an overestimation of the vanilla-note. From a quantitative point of view, there is probably too much vanillin already present due to the aromatization so that the minor additional amounts originating from the milk (more than 100-fold lower than in the strawberry aroma, 24) cannot be expected to play any significant sensory role. Generally, the difference between the overall aroma impressions of both samples (water and milk) was rated with 2.8 on the 0.0 to 3.0 scale as very high.
BOSS

Water Sample

In Figure 6, the results obtained from BOSS-analysis of the aqueous strawberry aroma sample are displayed in comparison to the retronasal odor threshold values of the respective compounds in water. It can be seen that BOSS-Screening of the oral cavity for potent odorants after exposure to the aromatized water sample led to the detection of most of the strawberry aroma constituents at the start point of analysis (15 sec). Interestingly, only the two compounds with the lowest retronasal odor threshold values were not detectable 15 sec after expectoration of the solution. This does not exclude that detection would be positive at an earlier stage of intraoral release (for example immediately after swallowing), but has not been further investigated.

When comparing the ROT-values with the total duration of detection by BOSS, it becomes evident that ROTV does not allow any prediction of intra-oral persistence. For example, ethyl butanoate with the by far highest ROTV of 360000 was intraorally only detectable for 2 min while vanillin and 2,5-dimethyl-4-hydroxy-3(2H)-furanone with the comparatively low ROTV of 67 could be found even after a period of eight minutes after expectoration. Therefore, apart from concentration and aroma intensity, factors such as polarity, volatility and stability in the presence of salivary constituents might be some factors being involved in this observation. Also, it has to be taken into account that odor intensity does not follow a straight correlation with increase of odor quantity but that it should be subjected to psychophysical phenomena as described by Stevens law (25). Therefore, the immediate retronasal aroma detection at ROTV-level (see also above “validation of detection”) is not at all comparable to long-time persistence, intensity and detectability of odorants at suprathreshold levels. However, it still has to be regarded as surprising that there is obviously so little relation between ROT-values and intra-oral detectability by BOSS. This experience has also been made in sensory evaluations, which will be reported elsewhere (26).

Generally, the grassy compounds hexanal and (Z)-3-hexenol, as well as the fruity compounds ethyl butanoate, ethyl isopentanoate, ethyl hexanoate, (Z)-3-hexenyl acetate, as well as methyl dihydrojasmonate were detectable by BOSS only for a relatively short period of time (up to 2 min), while the sweet and flowery compounds β-ionone, methyl cinnamate, methyl anthranilate and the coconut-like δ-decalactone
were even detectable after 4 and 8 min, respectively. In addition, vanillin and 2,5-dimethyl-4-hydroxy-3(2H)-furanone yielded this long duration of detection. Direct comparison of these observations to the sensorically perceived changes in aroma profile after consumption of the aqueous strawberry aroma sample (Figure 5) poses some difficulties. It becomes evident that for example the sensory persistence of the vanilla and the caramel note was only rated up to 2 and 4 min, respectively. However, the flowery impression was described by the panelists as very intense and dominant from the start point on. Therefore, it might be assumed that other odor notes were just covered by this impression. Furthermore, all these aroma impressions are very much related in their overall aroma character so that differentiation between them might cause some difficulties. On the other hand, the considerably correlated fit between the BOSS-detection of the grassy compounds (up to 2 min), the fruity (up to 2 min) and the flowery substances (8 min) and their corresponding duration of sensory perception (2 min, 4 min and 8 min, respectively) gives evidence of the capability of the BOS-System to screen odorants intraorally for their contribution in "afterodor" perception.

Milk sample
The significantly decreased intensities of the rated odor qualities in the strawberry flavoured milk sample (cf. Figure 4 and Figure 5) were also observable when evaluating the persistence of the single compounds by BOSS (cf. Figure 7). Mainly the flowery-sweet odorants, as well as 2,5-dimethyl-4-hydroxy-3(2H)-furanone and vanilllin were significantly reduced in their detectability, but also for the fruity esters and the grassy compounds differences could be observed. Again, complete correlation to the sensory perception is difficult, as there are probably additive or competitive effects. Moreover, it has to be taken into account that in the milk samples the milk-related odor notes were perceived additionally. This might explain why for example the flowery, caramel and vanilla notes were only perceivable for 1 or 2 min, respectively, while the BOSS analysis led to a detection at 2 or 4 min, respectively. However, the trend of matrix interaction could clearly be traced, so that the applicability as intraoral screening system was also demonstrated for a complex matrix system.
Chardonnay Wines

In the previous chapter, matrix effects on odorants were elucidated by means of BOSS-analysis and sensory evaluation. In this case, no real changes in the concentrations of the odorants occurred.

Subsequently, another application of the BOS-System shall be introduced: Two chardonnay wines, which exhibited considerable sensory differences, were profiled by sensory as well as by BOSS analysis. In parallels, quantisation of the potent odorants of the wines were performed by stable isotope dilution assays.

Sensory Evaluation

For comparison, both wines were evaluated retronasally according to selected odor descriptors as described in Sensory Evaluation, following the "time dilution" approach. At each evaluation time, the overall odor intensities were also rated. The profiles representing the intensities of the single odor qualities are given as spider web diagrams in Figure 8, together with a small bar diagram comparing the respective perceived overall intensities.

When looking at the overall intensities, an interesting phenomenon can be observed: at the beginning of the evaluation, both wines were rated with a similarly high intensity, slightly decreasing during the next 15 seconds. Then, a shift in intensity was detected, with the intensity of the Forest Hill wine decreasing more rapidly. However, the rating of the single odor qualities shows that these overall intensities cannot be simply related to the same aroma impressions. On the contrary, both aroma profiles differed considerably. From the start of the evaluation, the Forest Hill chardonnay was described as much more fruity, flowery, pungent and citrusy, while the Merryvale wine was dominated by woody, smoky, vanilla- and clove-like impressions. This general deviation remained more or less the same for the following evaluations, only with decreasing intensities. It has to be stated, that the fruity, flowery, pungent and citrusy decreased faster than the presumably barrique-related descriptors of the Merryvale wine. This explains the shift in the overall aroma intensities of both wines over the time course of evaluation.

Identification of the Potent Wine Odorants in Solvent Extracts

As wine aroma is a complex composition of a diversity of aroma compounds, the potent odorants of both wines were first isolated by means of solvent extraction, high vacuum distillation, concentration procedures and subsequent evaluation by means
of gas chromatography-olfactometry as well as mass spectrometry as described in the Experimental Chapter.
This approach led to the identification of a total of 33 potent odorants in both wines. These compounds, together with their odor qualities and retention indices are given in Table 6. Generally, most of the odorants were detectable in both wines. Only cis- and trans whiskey lactone and eugenol were not perceived in the Forest Hill sample, while on the other hand 3-methylbutyl acetate was not sensorically detectable in the Merryvale wine.

Comparative BOSS Analysis
Subsequent screening of both wines by means of comparative BOSS analysis using the "time dilution" approach led to the detection of most of the odorants which were previously found by HRGC/O of the solvent extracts (Figure 9). Only acetic, butanoic and phenylacetic acid, as well as methionol and abhexone were not perceived. Probable reasons are that these substances are quite polar and, on the other hand, the buffering capacity of the saliva is very high so that the acidic compounds should be mainly present in the deprotonated form. However, this has not been investigated in the present work. On the other hand, the concentrations of these compounds might be sufficient for detection in the concentrated solvent extracts obtained from 100 mL of the respective wines (see Experimental), but not high enough to be of retronasal sensory relevance (see below, Quantitation of the Potent Wine Odorants). Apart from these compounds, most odorants were detectable in both wines at the starting point of BOSS evaluation (15 sec after swallowing). The only exceptions were sotolone, eugenol, 2-methoxyphenol, cis- and trans-whiskey lactone and methional, which were only detectable after consumption of the Merryvale wine, while 3-methylbutyl acetate was missing here.
When looking at the total durations of detection of the remaining odorants, some significant differences become evident. First, vanillin and butan-2,3-dione were much longer detectable after intra-oral application of the Merryvale wine, and also (just by one TD step) phenylethanol, geraniol and ethyl 3-methylbutanoate, as compared to Forest Hill. In contrast to this, the persistence of β-ionone, phenylacetaldehyde and decanal was a bit reduced for Merryvale, but always just by one TD step.
The correlation of these observations to the sensory evaluation is striking. Both BOSS profiles mirror the higher persistence of woody, smoky, vanilla- and clove-like
odor notes from Merryvale wine (mainly represented by vanillin, eugenol, 2-methoxyphenol and the whiskeylactones). On the other hand, the more fruity, flowery, citrusy impressions should be not only explainable by the higher persistence of β-ionone, phenylacetaldehyde and decanal and the additional detection of 3-methylbutyl acetate, but also by the lower intensities of the above-mentioned woody, smoky, vanilla- and clove-like qualities. For these detection differences, several explanations are possible. First of all, that both wines simply contain different amounts of the respective odorants, resulting in higher intensities and persistences. This will be discussed in the following chapter. Also, there might be differences in the matrix composition of the wines so that the intra-oral release parameters might be changed. In this context, it also has to be mentioned that the ethanol content of both wines was not completely equal (Merryvale 14.5 % by vol., Forest Hill 13.5 % by vol.). Whether this difference has an effect e.g. on odorant-mucosa interactions and, as a consequence, on retronasal perceptibility with time, needs to be further investigated.

Quantitation of the Potent Wine Odorants

As discussed above, the question occurred whether both wines differed in the contents of some key odorants. To clarify this, 23 of the identified odorants were selected according to their odor intensities during gaschromatographic-olfactometric intensities (data not shown) and according to the differences observed in Comparative BOSS-analysis. Quantitation was performed by means of stable isotope dilution assays as described in the Experimental part.

Table 7 shows the concentrations of these odorants in both wines together with the respective mass traces analysed in SIDA.

A direct correlation was found for a series of substances between the quantitative data and the BOSS detection. First of all, considerably higher amounts of the whiskeylactones were found in the Merryvale wine with about 13 and 19-fold higher concentrations, respectively, than in Forest Hill. But also vanillin, eugenol, furaneol and 2-methoxyphenol were increased by a factor of about five. Apart from this, about two-fold higher concentrations were detected for ethyl 3-methylbutanoate, phenylethanol and ethyl cinnamate, while the amounts of 3-methylbutyl acetate were lower by a factor of about five than in Forest Hill. All these differences might have been expectable from the BOSS results, only for furaneol no increase in persistence
was found. The reasons for this are not yet fully clear. However, the concentrations in both wines were very low (for a comparison see the data of strawberry aroma with considerably higher amounts of furaneol), only resulting in detection at 15 sec and were probably not high enough to cause any significant effect in terms of persistence. There might have been just enough traces of wine back in the oral cavity to lead to detection but possibly there was not yet a real release from oral mucosa. It has to be stated here, that from the quantitative data it cannot be excluded that additional matrix effects occur, as discussed above. This will be elucidated by further model experiments, where wine solids will be isolated, recomposed according to the respective requirements and exposed to changing aroma compositions. This approach will lead to a fundamental understanding of aroma release under in vivo conditions and, which is much more important, in real-food concentrations.

Summarising the results of the quantisation experiments, a perfect correlation between the most potent odorants of both wines, the detectability via BOSS analysis and the perception of retronasal intensities of odor qualities with time has been achieved. Again, this was a convincing proof of the validity of the BOSS approach to profile retronasal aroma perception as a function of the composition of the food aroma and the food matrix applied.

General Comments

The present study shows that BOSS leads to an array of applications. At first, afterodor characterization after food consumption by means of precise analytical terms is the obvious task. In this context, not only the development/decrease of desired but also of undesired smells (e.g. garlic, beer, cigarette smoke, etc.) can now be easily followed and traced back to the key odor active substances even at lowest concentrations.

Also, diverse matrix effects can be investigated which can be divided into different groups: for example direct aroma-matrix interactions which influence the release of odorants from the matrix itself, but also matrix-induced effects which modify the surface of the oral mucosa either by forming some kinds of coatings (as it has been reported elsewhere, 27) or by altering the general properties of the mucosa itself (see e.g. mouthwashes, oral treatments).

From an analytical point of view, the technique described herein offers, for the first time, the possibility to strike the balance of food odorants in-vivo. First, adsorption of
odorants to oral mucosa under precisely defined conditions can be quantified according to the SOOM-approach. Release therefrom into salivary and air phases present in the oral mucosa can now not only be detected but also quantified by exposing the stir bar after oral application to suitable standards preferably stable isotope labelled standards. Feasibility of this approach has already been proofed (unpublished data) and the validation of this technique and some in-vivo applications will be published soon. Apart from the quantisation of odorant adsorption to mucosa and the release therefrom, also the amounts being transferred to the olfactory area can now be not only be detected but also exactly quantified even in trace concentrations as it has been shown recently (28). In this approach, the volatiles including key odorants are collected from the nose (or mouth) by trapping the exhaled air. This can be achieved for example by cryofocusation as it was done previously using a glass tube or glass helix where the air is led through and which is immersed into liquid nitrogen (29). Other techniques such as TENAX-trapping as described previously in the EXOM-Approach are also possible (30). Collection of the trapped odorants from the frozen breath can be achieved for example by solvent uptake or also by introduction of e.g. an SBSE-bar into the aqueous breath phase or any other adsorptive device capable for collecting the respective odorants. If quantisation is planned to be performed, addition of the respective standard to the frozen or otherwise trapped breath is recommended (together with the respective equilibration times) prior to recollection by SBSE or any other technique. This quantisation setup has already been proofed to be successful in the investigation of beverages and will be published soon. Combining now all three analytical approaches draws a comprehensive picture of the fate of odorants on their retronasal way from the oral cavity to the nasal areas where they can reach the receptor sides. Once again it has to be stated, that this is, for the first time, possible under unchanged in-vivo conditions, for potent and relevant aroma compounds and, furthermore, in real-food odorant concentrations and under realistic matrix composition conditions.

The combination of the three techniques, quantisation of odorant adsorption to mucosa, release in the oral cavity and retronasal transfer to the nasal areas (allowing indirect quantisation of odorant losses on their way) will be soon published as an overall concept (31).
Leaving the food area and relating to other topics, one can transfer the technique to the detection of compounds which are related to the physical status of a person or are indicators of diseases. In the case of halitosis for example (a problem which has not yet been fully elucidated), the characterization of the odorous substances can give an idea of the origin of these substances. On the other hand, the effectiveness of remedies against these odors (decrease of off-odor substances upon treatment or just masking effects by other more potent, e.g. fresh compounds) can also be directly evaluated. However, not only odorous compounds need to be necessarily investigated. There might be also an applicability of this simply in-vivo (optionally also ex-vivo performed) approach to find other markers for diseases etc.

CONCLUSIONS AND OUTLOOK
The feasibility of the BOS-System to screen intraorally even traces of key odorants with regard to their retronasal aroma contribution and involvement in the phenomenon of "afterodor" or "aftersmell" has been demonstrated. Further applications involve the characterization of intra-oral odor or off-odor development. Some examples comprise smells arising after food consumption, after application of any kind of oral treatments, smoking, general medical treatment or odor-development in relation to the respective physiological status, diseases (see halitosis phenomena), etc. Furthermore, the effects of counter-actions taken, such as application of mouthwashes, etc., can be directly followed not only by sensory evaluation but also by precise analytical terms.
Table 1. Strawberry Aroma Composition and Final Concentrations of the Single Constituents in the Water and Milk Samples.

<table>
<thead>
<tr>
<th>Odorant</th>
<th>Odor Quality</th>
<th>Concentration [mg/L]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethyl butanoate</td>
<td>fruity</td>
<td>36</td>
</tr>
<tr>
<td>Ethyl 3-methylbutanoate</td>
<td>fruity</td>
<td>4</td>
</tr>
<tr>
<td>Ethyl hexanoate</td>
<td>fruity</td>
<td>8</td>
</tr>
<tr>
<td>(Z)-3-Hexenyl acetate</td>
<td>fruity</td>
<td>2</td>
</tr>
<tr>
<td>Methyl cinnamate</td>
<td>sweet</td>
<td>9.6</td>
</tr>
<tr>
<td>Styrallyl acetate</td>
<td>sweet</td>
<td>0.4</td>
</tr>
<tr>
<td>Benzyl acetate</td>
<td>sweet</td>
<td>0.8</td>
</tr>
<tr>
<td>Methyl anthranilate</td>
<td>sweet</td>
<td>0.4</td>
</tr>
<tr>
<td>Methyl dihydrojasmonate</td>
<td>fresh, fruity</td>
<td>2</td>
</tr>
<tr>
<td>γ-Decalactone</td>
<td>coconut-like</td>
<td>8</td>
</tr>
<tr>
<td>Hexanal</td>
<td>grassy</td>
<td>0.4</td>
</tr>
<tr>
<td>(Z)-3-Hexenol</td>
<td>grassy</td>
<td>6</td>
</tr>
<tr>
<td>β-Ionone</td>
<td>violet-like</td>
<td>0.4</td>
</tr>
<tr>
<td>2,5-Dimethyl-4-hydroxy-3(2H)-furanone</td>
<td>caramel-like</td>
<td>2</td>
</tr>
<tr>
<td>Vanillin</td>
<td>vanilla-like</td>
<td>2</td>
</tr>
</tbody>
</table>
Table 2. PDMS-Coating Parameters.

<table>
<thead>
<tr>
<th>No.</th>
<th>SBSE-Bar Length [mm]</th>
<th>Thickness of Coating [mm]</th>
<th>Total PDMS Volume [µL]</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>10</td>
<td>0.5</td>
<td>24</td>
</tr>
<tr>
<td>B</td>
<td>10</td>
<td>1</td>
<td>63</td>
</tr>
<tr>
<td>C</td>
<td>20</td>
<td>0.5</td>
<td>47</td>
</tr>
<tr>
<td>D</td>
<td>20</td>
<td>1</td>
<td>126</td>
</tr>
</tbody>
</table>
Table 3. Odorants Detectable by the SBSE-System after Conditioning.

<table>
<thead>
<tr>
<th>Odorant</th>
<th>Odor Quality</th>
<th>Retention Index a on FFAP</th>
<th>SE-54</th>
<th>OTV b [ng/L air] b</th>
</tr>
</thead>
<tbody>
<tr>
<td>Butane-2,3-dione</td>
<td>buttery</td>
<td>970</td>
<td>&lt;600</td>
<td>15-30</td>
</tr>
<tr>
<td>[Octanal]</td>
<td>citrus-like</td>
<td>1279</td>
<td>1000</td>
<td>5.8-13.6</td>
</tr>
<tr>
<td>Oct-1-en-3-one</td>
<td>mushroom-like</td>
<td>1295</td>
<td>976</td>
<td>0.3-0.6</td>
</tr>
<tr>
<td>[Acetic acid]</td>
<td>acidic</td>
<td>1449</td>
<td>610</td>
<td>60</td>
</tr>
<tr>
<td>[Methional]</td>
<td>cooked potato</td>
<td>1449</td>
<td>900</td>
<td>0.1-0.2</td>
</tr>
<tr>
<td>(E)-2-Nonenal</td>
<td>fatty, tallowy</td>
<td>1527</td>
<td>1157</td>
<td>0.1-0.2</td>
</tr>
<tr>
<td>3-Methylbutanoic acid</td>
<td>sweaty</td>
<td>1660</td>
<td>875</td>
<td>1.5</td>
</tr>
<tr>
<td>[β-Damascenone]</td>
<td>apple-like</td>
<td>1819</td>
<td>1389</td>
<td>0.002-0.004</td>
</tr>
<tr>
<td>tr-4,5-Epoxy-(E)-2-decenal</td>
<td>metallic</td>
<td>2000</td>
<td>1380</td>
<td>0.0006-0.0025</td>
</tr>
<tr>
<td>2,5-Dimethyl-4-hydroxy-3(2H)-furanone</td>
<td>caramel-like</td>
<td>2024</td>
<td>1062</td>
<td>1.0-2.0</td>
</tr>
<tr>
<td>Vanillin</td>
<td>vanilla-like</td>
<td>2567</td>
<td>1397</td>
<td>0.6-1.2</td>
</tr>
</tbody>
</table>

a Retention indices were calculated according to (32).

b The odor threshold values in air were determined as described elsewhere (33).
Table 4. Detection of Odorants in the Oral Cavity of a Healthy Panelist Prior to Food Consumption (Blank).

<table>
<thead>
<tr>
<th>No.</th>
<th>Odorant</th>
<th>Odor Quality</th>
<th>Retention Index $^a$ on</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>FFAP</td>
</tr>
<tr>
<td>1</td>
<td>Oct-1-en-3-one</td>
<td>mushroom-like</td>
<td>1295</td>
</tr>
<tr>
<td>2</td>
<td>Acetic acid</td>
<td>acidic</td>
<td>1449</td>
</tr>
<tr>
<td>3</td>
<td>Methional</td>
<td>cooked potato</td>
<td>1449</td>
</tr>
<tr>
<td>4</td>
<td>(Z)-2-Nonenal</td>
<td>fatty, leaf-like</td>
<td>1502</td>
</tr>
<tr>
<td>5</td>
<td>(E)-2-Nonenal</td>
<td>fatty, tallowy</td>
<td>1527</td>
</tr>
<tr>
<td>6</td>
<td>(E,Z)-2,6-Nonadienal</td>
<td>cucumber-like</td>
<td>1583</td>
</tr>
<tr>
<td>7</td>
<td>unknown</td>
<td>green coriander</td>
<td>~2400</td>
</tr>
<tr>
<td>8</td>
<td>3-Methyldindole</td>
<td>faeces-like</td>
<td>2484</td>
</tr>
</tbody>
</table>

$^a$ Retention indices were calculated according to (32).
<table>
<thead>
<tr>
<th>Odorant</th>
<th>Odor Quality</th>
<th>ROTV</th>
<th>Detection at</th>
<th>MW</th>
<th>logP&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethyl isobutanoate</td>
<td>fruity</td>
<td>0.03</td>
<td>+</td>
<td>-</td>
<td>116 3.00</td>
</tr>
<tr>
<td>3-Methylbutanal</td>
<td>malty</td>
<td>0.04</td>
<td>+</td>
<td>-</td>
<td>86   1.29</td>
</tr>
<tr>
<td>Methional</td>
<td>cooked potato</td>
<td>0.04</td>
<td>(+)</td>
<td>-</td>
<td>104 0.87</td>
</tr>
<tr>
<td>Butane-2,3-dione</td>
<td>buttery</td>
<td>0.2</td>
<td>+</td>
<td>not determ.</td>
<td>86   1.67</td>
</tr>
<tr>
<td>Pentane-2,3-dione</td>
<td>buttery</td>
<td>5</td>
<td>+</td>
<td>-</td>
<td>100 2.19</td>
</tr>
<tr>
<td>Oct-1-en-3-one</td>
<td>mushroom-like</td>
<td>0.01</td>
<td>+</td>
<td>not determ.</td>
<td>126 2.22</td>
</tr>
<tr>
<td>2-Ethyl-3,5-dimethylpyrazine</td>
<td>earthy</td>
<td>0.08</td>
<td>+</td>
<td>-</td>
<td>136 1.82</td>
</tr>
<tr>
<td>3-Isobutyl-2-methoxypyrazine</td>
<td>pea-like</td>
<td>0.005</td>
<td>(+)</td>
<td>-</td>
<td>166 1.89</td>
</tr>
<tr>
<td>Furfurylthiol</td>
<td>coffee-like</td>
<td>0.005</td>
<td>+</td>
<td>-</td>
<td>114 0.86</td>
</tr>
<tr>
<td>Butanoic acid</td>
<td>sweaty</td>
<td>1000</td>
<td>+</td>
<td>-</td>
<td>88   1.87</td>
</tr>
<tr>
<td>2-Phenylethanol</td>
<td>flowery</td>
<td>45</td>
<td>+</td>
<td>-</td>
<td>122 1.49</td>
</tr>
<tr>
<td>2-Methoxyphenol</td>
<td>smoky</td>
<td>0.75</td>
<td>+</td>
<td>-</td>
<td>124 1.62</td>
</tr>
<tr>
<td>2-Methoxy-4-vinylphenol</td>
<td>clove-like</td>
<td>5</td>
<td>+</td>
<td>-</td>
<td>150 2.47</td>
</tr>
<tr>
<td>β-Damascenone</td>
<td>cooked apple</td>
<td>0.001</td>
<td>+</td>
<td>not determ.</td>
<td>190 4.03</td>
</tr>
<tr>
<td>Ethyl butanoate</td>
<td>fruity</td>
<td>0.1</td>
<td>+</td>
<td>-</td>
<td>116 3.00</td>
</tr>
<tr>
<td>Ethyl 3-methylbutanoate</td>
<td>fruity</td>
<td>0.1</td>
<td>+</td>
<td>-</td>
<td>130 3.52</td>
</tr>
<tr>
<td>Compound</td>
<td>Description</td>
<td>Value 1</td>
<td>Value 2</td>
<td>Value 3</td>
<td>Value 4</td>
</tr>
<tr>
<td>--------------------------------</td>
<td>-----------------</td>
<td>---------</td>
<td>---------</td>
<td>---------</td>
<td>---------</td>
</tr>
<tr>
<td>Ethyl hexanoate</td>
<td>fruity</td>
<td>0.6</td>
<td>+</td>
<td>-</td>
<td>144</td>
</tr>
<tr>
<td>(Z)-3-Hexenyl acetate</td>
<td>fruity</td>
<td>12.1</td>
<td>+</td>
<td>-</td>
<td>142</td>
</tr>
<tr>
<td>Methyl cinnamate</td>
<td>sweet</td>
<td>11</td>
<td>+</td>
<td>-</td>
<td>162</td>
</tr>
<tr>
<td>Styrraly acetate</td>
<td>sweet</td>
<td>39</td>
<td>+</td>
<td>-</td>
<td>164</td>
</tr>
<tr>
<td>Benzyl acetate</td>
<td>sweet</td>
<td>37</td>
<td>+</td>
<td>-</td>
<td>150</td>
</tr>
<tr>
<td>Methyl anthranilate</td>
<td>sweet</td>
<td>1.5</td>
<td>+</td>
<td>-</td>
<td>151</td>
</tr>
<tr>
<td>Methyl dihydrojasmonate</td>
<td>sweet</td>
<td>28</td>
<td>+</td>
<td>-</td>
<td>226</td>
</tr>
<tr>
<td>γ-Decalactone</td>
<td>coconut-like</td>
<td>88</td>
<td>+</td>
<td>+</td>
<td>170</td>
</tr>
<tr>
<td>Hexanal</td>
<td>grassy</td>
<td>10.5</td>
<td>+</td>
<td>-</td>
<td>100</td>
</tr>
<tr>
<td>(Z)-3-Hexenol</td>
<td>grassy</td>
<td>30</td>
<td>+</td>
<td>-</td>
<td>100</td>
</tr>
<tr>
<td>β-Ionone</td>
<td>violet-like</td>
<td>0.1</td>
<td>+</td>
<td>-</td>
<td>192</td>
</tr>
<tr>
<td>2,5-Dimethyl-4-hydroxy-3(2H)-furanone</td>
<td>caramel-like</td>
<td>30</td>
<td>+</td>
<td>-</td>
<td>128</td>
</tr>
<tr>
<td>Vanillin</td>
<td>vanilla-like</td>
<td>30</td>
<td>+</td>
<td>-</td>
<td>152</td>
</tr>
</tbody>
</table>

* logP values were calculated according to (34).
Table 6. Odorant Detection in Solvent Extracts of two Chardonnay Wines by Means of HRGC/O.

<table>
<thead>
<tr>
<th>Odorant</th>
<th>Forest Hill</th>
<th>Merryvale</th>
<th>Odor Quality</th>
<th>Retention Index on FFAP a</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 2-3-Methylbutanal</td>
<td>+</td>
<td>+</td>
<td>malty</td>
<td>0913</td>
</tr>
<tr>
<td>2 Ethanol</td>
<td>+</td>
<td>+</td>
<td>ethanolic</td>
<td>0930</td>
</tr>
<tr>
<td>3 Ethyl methylpropanoate</td>
<td>+</td>
<td>+</td>
<td>fruity</td>
<td>0955</td>
</tr>
<tr>
<td>4 Butane-2,3-dione</td>
<td>+</td>
<td>+</td>
<td>buttery</td>
<td>0981</td>
</tr>
<tr>
<td>5 Ethyl butanoate</td>
<td>+</td>
<td>+</td>
<td>fruity</td>
<td>1028</td>
</tr>
<tr>
<td>6 Ethyl 2/3-methylbutanoate</td>
<td>+</td>
<td>+</td>
<td>fruity</td>
<td>1041</td>
</tr>
<tr>
<td>7 3-Methylbutyl acetate</td>
<td>+</td>
<td>-</td>
<td>banana-like</td>
<td>1117</td>
</tr>
<tr>
<td>8 2-3-Methylbutanol</td>
<td>+</td>
<td>+</td>
<td>malty</td>
<td>1211</td>
</tr>
<tr>
<td>9 Ethyl hexanoate</td>
<td>+</td>
<td>+</td>
<td>fruity</td>
<td>1226</td>
</tr>
<tr>
<td>10 Oct-1-en-3-one</td>
<td>+</td>
<td>+</td>
<td>mushroom-like</td>
<td>1295</td>
</tr>
<tr>
<td>11 Acetic acid</td>
<td>+</td>
<td>+</td>
<td>acetic</td>
<td>1449</td>
</tr>
<tr>
<td>12 Methional</td>
<td>+</td>
<td>+</td>
<td>potato-like</td>
<td>1449</td>
</tr>
<tr>
<td>13 Decanal</td>
<td>+</td>
<td>+</td>
<td>citrus, soapy</td>
<td>1493</td>
</tr>
<tr>
<td>14 Butanoic acid</td>
<td>+</td>
<td>+</td>
<td>sweaty</td>
<td>1619</td>
</tr>
<tr>
<td>15 Phenylacetaldehyde</td>
<td>+</td>
<td>+</td>
<td>honey-like</td>
<td>1639</td>
</tr>
<tr>
<td>16 3-Methylbutanoic acid</td>
<td>+</td>
<td>+</td>
<td>sweaty</td>
<td>1661</td>
</tr>
<tr>
<td>17 Methionol</td>
<td>+</td>
<td>+</td>
<td>potato-like</td>
<td>1705</td>
</tr>
<tr>
<td>18 β-Damascenone</td>
<td>+</td>
<td>+</td>
<td>cooked apple</td>
<td>1810</td>
</tr>
<tr>
<td>19 Geraniol</td>
<td>+</td>
<td>+</td>
<td>fresh, fruity</td>
<td>1818</td>
</tr>
<tr>
<td>20 trans-Whiskeylactone</td>
<td>-</td>
<td>+</td>
<td>coconut-like</td>
<td>1830</td>
</tr>
<tr>
<td>21 2-Methoxyphenol</td>
<td>(+)</td>
<td>+</td>
<td>smoky</td>
<td>1859</td>
</tr>
<tr>
<td>22 Phenylethanol</td>
<td>+</td>
<td>+</td>
<td>honey-like</td>
<td>1860</td>
</tr>
<tr>
<td>23 β-Ionone</td>
<td>+</td>
<td>+</td>
<td>violet-like</td>
<td>1920</td>
</tr>
<tr>
<td>24 cis-Whiskeylactone</td>
<td>-</td>
<td>+</td>
<td>coconut-like</td>
<td>1920</td>
</tr>
<tr>
<td>25 2,5-Dimethyl-4-hydroxy-3(2H)-furanone</td>
<td>+</td>
<td>+</td>
<td>caramel-like</td>
<td>2031</td>
</tr>
<tr>
<td>26 Ethylcinnamat</td>
<td>+</td>
<td>+</td>
<td>flowery, sweet</td>
<td>2123</td>
</tr>
<tr>
<td></td>
<td>Compound</td>
<td>-</td>
<td>+</td>
<td>Description</td>
</tr>
<tr>
<td>---</td>
<td>---------------------------------</td>
<td>---</td>
<td>---</td>
<td>-----------------</td>
</tr>
<tr>
<td>27</td>
<td>Eugenol</td>
<td></td>
<td>+</td>
<td>smoky</td>
</tr>
<tr>
<td>28</td>
<td>δ-Decalactone</td>
<td>+</td>
<td>+</td>
<td>coconut-like</td>
</tr>
<tr>
<td>29</td>
<td>Sotolone</td>
<td>+</td>
<td>+</td>
<td>spicy</td>
</tr>
<tr>
<td>30</td>
<td>2-Methoxy-4-vinylphenol</td>
<td>+</td>
<td>+</td>
<td>clove-like</td>
</tr>
<tr>
<td>31</td>
<td>Abhexon</td>
<td>+</td>
<td>+</td>
<td>spicy</td>
</tr>
<tr>
<td>32</td>
<td>Phenyl acetic acid</td>
<td>+</td>
<td>+</td>
<td>honey-like</td>
</tr>
<tr>
<td>33</td>
<td>Vanillin</td>
<td>+</td>
<td>+</td>
<td>vanilla-like</td>
</tr>
</tbody>
</table>

* Retention indices were calculated according to (32).
Table 7. Concentrations of Potent Odorants in two Chardonnay White Wines and the Respective Mass Traces used for Quantitation.

<table>
<thead>
<tr>
<th>Odorant</th>
<th>Forest Hill</th>
<th>Merryvale</th>
<th>Unlabeled</th>
<th>Labelled</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 2-/3-Methylbutanal</td>
<td>nd</td>
<td>nd</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>2 Ethanol</td>
<td>nd</td>
<td>nd</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>3 Ethyl methylpropanoate</td>
<td>72.2</td>
<td>99.9</td>
<td>117</td>
<td>120</td>
</tr>
<tr>
<td>4 Butane-2,3-dione</td>
<td>nd</td>
<td>172.7</td>
<td>87</td>
<td>91</td>
</tr>
<tr>
<td>5 Ethyl butanoate</td>
<td>263.0</td>
<td>341.5</td>
<td>117</td>
<td>120</td>
</tr>
<tr>
<td>6 Ethyl 2/3-methylbutanoate</td>
<td>9.2</td>
<td>19.9</td>
<td>131</td>
<td>134</td>
</tr>
<tr>
<td>7 3-Methylbutyl acetate</td>
<td>943.7</td>
<td>163.5</td>
<td>131</td>
<td>133</td>
</tr>
<tr>
<td>8 3-Methylbutanol</td>
<td>253591</td>
<td>356725</td>
<td>71</td>
<td>73</td>
</tr>
<tr>
<td>9 Ethyl hexanoate</td>
<td>757.2</td>
<td>737.5</td>
<td>145</td>
<td>148</td>
</tr>
<tr>
<td>10 Oct-1-en-3-one</td>
<td>nd</td>
<td>nd</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>11 Acetic acid</td>
<td>434232</td>
<td>489370</td>
<td>61</td>
<td>63</td>
</tr>
<tr>
<td>12 Methional</td>
<td>nd</td>
<td>nd</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>13 Decanal</td>
<td>20.0</td>
<td>15.3</td>
<td>157</td>
<td>158-160</td>
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<tr>
<td>14 Butanoic acid</td>
<td>1839</td>
<td>1611</td>
<td>89</td>
<td>91</td>
</tr>
<tr>
<td>15 Phenylacetaldehyde</td>
<td>nd</td>
<td>nd</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>16 3-Methylbutanoic acid</td>
<td>588.0</td>
<td>561.6</td>
<td>103</td>
<td>105</td>
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<tr>
<td>17 Methionol</td>
<td>563.4</td>
<td>795.6</td>
<td>107</td>
<td>110</td>
</tr>
<tr>
<td>18 β-Damascenone</td>
<td>nd</td>
<td>nd</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>19 Geraniol</td>
<td>nd</td>
<td>nd</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>20 trans-Whiskeylactone</td>
<td>7.1</td>
<td>131.1</td>
<td>157</td>
<td>159</td>
</tr>
<tr>
<td>21 2-Methoxyphenol</td>
<td>2.7</td>
<td>9.9</td>
<td>125</td>
<td>128</td>
</tr>
<tr>
<td>22 Phenylethanol</td>
<td>12415</td>
<td>24971</td>
<td>105</td>
<td>107</td>
</tr>
<tr>
<td>23 β-Ionone</td>
<td>nd</td>
<td>nd</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>24 cis-Whiskeylactone</td>
<td>17.0</td>
<td>214.8</td>
<td>157</td>
<td>159</td>
</tr>
<tr>
<td>25 2,5-Dimethyl-4-hydroxy-3(2H)-furanone</td>
<td>2.1</td>
<td>13.7</td>
<td>129</td>
<td>131</td>
</tr>
<tr>
<td>No.</td>
<td>Substance</td>
<td>Value1</td>
<td>Value2</td>
<td>Value3</td>
</tr>
<tr>
<td>-----</td>
<td>----------------------------------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>26</td>
<td>Ethylcinnamat</td>
<td>1.5</td>
<td>3.1</td>
<td>177</td>
</tr>
<tr>
<td>27</td>
<td>Eugenol</td>
<td>1.6</td>
<td>8.9</td>
<td>165</td>
</tr>
<tr>
<td>28</td>
<td>δ-Decalactone</td>
<td>30.4</td>
<td>32.4</td>
<td>171</td>
</tr>
<tr>
<td>29</td>
<td>Sotolone</td>
<td>nd</td>
<td>nd</td>
<td>---</td>
</tr>
<tr>
<td>30</td>
<td>2-Methoxy-4-vinylphenol</td>
<td>50.5</td>
<td>49.3</td>
<td>151</td>
</tr>
<tr>
<td>31</td>
<td>Abhexon</td>
<td>nd</td>
<td>nd</td>
<td>---</td>
</tr>
<tr>
<td>32</td>
<td>Phenyl acetic acid</td>
<td>34.6</td>
<td>90.0</td>
<td>137</td>
</tr>
<tr>
<td>33</td>
<td>Vanillin</td>
<td>48.5</td>
<td>241.6</td>
<td>153</td>
</tr>
</tbody>
</table>
Enantiomer, & Odor Description

Cyclic, Terpenoid, Odorants

(R)-(+) - limonene, fresh, citrus, orange-like
(S)-(+) - limonene, harsh, turpentine-like, lemon note
(R)-(+) - alpha-phellandrene, terpene-like, medicinal
(S)-(+) - alpha-phellandrene, characteristic, dill note
(S)-(+) - alpha-terpineol, coniferous, odor, tarry, cold, pipe, like
(R)-(+) - alpha-terpineol, heavy, floral, lilac-like, odor

(1R, 3R, 4S)-(-)-menthol, cooling, fresh, sweet, minty
(1S, 3R, 4R)-(+)-menthol, fresh, some, cooling, sweet-minty with musty, bitter, phenolic, and herbaceous notes
(1R, 3S, 4S)-(-)-neomenthol, sweet, musty, fresh, some, cooling, minty
(1S, 3R, 4R)-(-)-neomenthol, minty, musty, fresh, earthy, camphoraceous, some, cooling
(1R, 3S, 4R)-(-)-isomenthol, -musty, woody, fresh, carrot-minty, earthy, camphoraceous, slight, cooling
(1S, 3R, 4S)-(+)-isomenthol, -musty, sweet, herbaceous, earthy, camphoraceous, hay, slight, cooling
(1S, 3S, 4S)-(-)-neoisomenthol, -musty, earthy, camphoraceous, sweet, minty, woody, slight, cooling
(1R, 3R, 4R)-(+)-neoisomenthol, -musty, earthy, camphoraceous, woody, carrot, herbaceous, minty, very little, cooling

(4R, 2S)-(-)-cis-rose oxide, -floral, green, with clean, sharp, light, rose, green note, diffusive, strong, also has been described as powerful, fruity
(4S, 2R)-(+)-cis-rose oxide, -herbal, green, floral, hay, green, earthy, heavy, also has been described as sweet, floral
(4R, 2R)-(-)-trans-rose oxide, -floral, green, herbal, minty, fruity
(4S, 2S)-(+)-trans-rose oxide, -herbal, green, floral fruit, herbal, rose, citrus (bitter, peel)
(4S, 2S)-(+)-cis-di-hydro rose oxide, -floral, green, clean, light, ripe, fruit, rose, green, and leafy, note, (Matsuda)
(4R, 2R)-(-)-cis-di-hydro rose oxide, -herbal, green, herbal, leafy, green, heavy, (Matsuda)
(4R, 2S)-(+)-trans-di-hydro rose oxide, -herbal, floral, fruity, minty, dusty, floral, green, (Matsuda)
(4S, 2R)-(+)-trans-di-hydro rose oxide, -herbal, green, citrus, fruity, herbal, fresh, citrus, (grapefruit), (Matsuda)

(S)-(-)-nerol oxide, -green, spicy, geranium
(R)-(+) - nerol oxide, -green, floral, less complex than, the, (S)-isomer
(4R)-(-)-carvone, -Swee, spearmint, fresh, herbal
(4S)-(-)-carvone, -caraway, fresh, herbal
(5)-(+) - 1-p-menth-8-thiol, -grapefruit, possessed, a more, fruity, and less, sulfur, note, than, its, (R)-(+) - enantiomer
(1R, 4R)-trans-p-menth-8-thiol-3-one, -onion-like, weak, fruity, tropical, dirty
(1S, 4S)-trans-p-menth-8-thiol-3-one, -stronger, than, (1R, 4R)-

isomer, tropical, sulfurous, pronounced, bchu, leaf, oil, notes
(1S, 4R)-cis-p-menth-8-thiol-3-one, -black, currant, leaf, tropical, note, of, passion, fruit, intensive, fruit, note
(1R, 4S)-cis-p-menth-8-thiol-3-one, -rubber, mercaptan, note, isopulegone, note, burnt, sulfurious, disagreeable
(4S)-(-)-terpinen-4-ol, -musty, dusty, (odor, evaluation, by, GC-olfactometry)
(4R)-(+) -terpinen-4-ol, -musty, (odor, evaluation, by, GC-olfactometry)
(3R, 6R)-cis-linalool oxide, (pyranoid), -earthy
(3S, 6S)-cis-linalool oxide, (pyranoid), -sweet, floral, creamy
(2R, 5S)-cis-linalool oxide, (furanoïd), -leafy, earthy
(2S, 5R)-cis-linalool oxide, (furanoïd), -sweet, floral, creamy
(2R, 5R)-trans-linalool oxide, (furanoïd), -leafy, earthy
(2S, 5S)-trans-linalool oxide, (furanoïd), -sweet, floral, creamy
(2S, 2'S, 5'S)-Lilac, aldehyde, -fresh, flowery
(2R, 2'R, 5'R)-Lilac, aldehyde, -flowery
(2R, 2'S, 5'S)-Lilac, aldehyde, -pleasant, flowery, fresh
(2S, 2'R, 5'R)-Lilac, aldehyde, -flowery
(2S, 2'R, 5'S)-Lilac, aldehyde, -sweet, flowery
(2R,2'S,5'R)-Lilac, aldehyde, -flowery, fresh
(2R,2'R,5'S)-Lilac, aldehyde, -sweet, flowery
(2S,2'S,5'R)-Lilac, aldehyde, -flowery, fresh
(2R,2'S,5'S)-Lilac, alcohol, -green, grassy, fresh
(2S,2'R,5'R)-Lilac, alcohol, -sweet
(2S,2'S,5'S)-Lilac, alcohol, -flowery
(2R,2'R,5'R)-Lilac, alcohol, -odorless, at >100 ng, by, GC, sniffing
(2R,2'R,5'S)-Lilac, alcohol, -flowery, sweet, body
(2S,2'S,5'R)-Lilac, alcohol, -herbaceous, slightly, flowery
(2S,2'S,5'S)-Lilac, alcohol, -sweet, flowery
(2R,2'S,5'R)-Lilac, alcohol, -sweet
(R)-(+) -Karahanaenol, -Both, enantiomers of, karahanaenol, have a, mint, like, odor, "The, (S)-enantiomer had a, notably, fresher, odor, than, the, (R).
(S)-(+) -Karahanaenol, -Both, enantiomers of, karahanaenol, have a, mint, like, odor, "The, (S)-enantiomer had a, notably, fresher, odor, than, the, (R).

Bicyclic, Terpenoid, Odorants
(1R,5R)-(+) -alpha-pinene, -harsh, terpene-like, minty
(1S,5S)-(+) -alpha-pinene, -harsh, terpene-like, coniferous
(R)-(+) -isoborneol, -camphoraceous, cellulosoid-like
(S)-(+) -isoborneol, -camphoraceous, sweet, & musty
(R)-(+) -2-methylisoborneol, -camphoraceous, rubbery
(S)-(+) -2-methylisoborneol, -camphoraceous, rubbery, also, described, as, musty, mold-like, earthy, by, Blank, & Grosh
(R)-(+) -2-methylborneol, -camphoraceous, rubbery
(S)-(+) -2-methylborneol, -camphoraceous, rubbery
(1R,4S)-(++) -fenchone, -camphoraceous, strong, diffusive, sweet, odor, for, racemate
(1S,4R)-(++) -fenchone, -camphoraceous, strong, diffusive, sweet, odor, for, racemate
(1R,4R)-(++) -camphor, -camphoraceous
(1S,4S)-(++) -camphor, -camphoraceous
(1S,4R,6S)-6-Acetoxy-1,8-cineole, -woody, (weak)
(1R,4S,6R)-6-Acet oxy-1,8-cineole, -woody, Alpinia galanga, like, and, stronger, than, the, (1S,4R,6S)-isomer
(1S,4R,6R)-6-Acet oxy-1,8-cineole, -weak
(1R,4S,6S)-6-Acet oxy-1,8-cineole, -fruity, sweet
(1S,4R,5R)-5-Acet oxy-1,8-cineole, -sweet, floral, weak, (virtually, to, weak, to, evaluate)
(1R,4S,5S)-5-Acet oxy-1,8-cineole, -sweet, floral, weak, (virtually, to, weak, to, evaluate)
(1S,4R,5R)-5-Acet oxy-1,8-cineole, -camphoraceous
(1R,4S,5R)-5-Acet oxy-1,8-cineole, -mild, woody
(1S,2R,4S)-(--) -borneol, (1S,2R,4S)-(--) -borneol, -camphoraceous, India, ink, like, slight, fatty, putrid, (odor, evaluation, by, GC-olfactometry), (Nishimura), camphoraceous, and, evident, woody, odor
(1R,2S,4R)-(++) -borneol, -camphoraceous, India, ink, like, (odor, evaluation, by, GC-olfactometry), (Nishimura), a, camphoraceous, odor, and, a, slightly, sharp, earthy, peppery, note, different, from, that, of, the, (--) form

Acyclic, Terpenoid, Odorants
(S)-(++) -linalool, -sweet, floral, odor, reminiscent, of, petitgrain, and, lavender
(R)-(--) -linalool, -floral, woody, lavender, note
(S)-(--) -citronellol, -floral, rose-like, odor, reminiscent, of, geranium, oil, Described, by, Yamamoto, et, al, as, very, fresh, light, and, clean, rosy-leafy, petal-like
(R)-(++) -citronellol, -citronella, oil, like, Described, by, Yamamoto, et, al, as, slightly, oily, light, rosy-leafy, petal, like, odor, with, irritating, top, note
(6S)-(--) -6,7-epoxygeraniol, -lactone, like, rosy
Ionones, Irones, Damascones, & Structurally Related Odorants

(R)-(+)-(E)-alpha-ionone, - violet-like, fruity, raspberry-like, flowery, strong impact
(S)-(--)-(E)-alpha-ionone, - woody, cedar, wood-like, raspberry, & beta-ionone like
(R)-(--)-(E)-gamma-ionone, - weak, green, fruity, pineapple-like, odor, with metallic aspects, quite different from the, typical ionone odor, however, slightly woody, ionone-type nuances are also, present.
(S)-(--)-(E)-alpha-ionone, -
 Linear, very pleasant, floral, green, woody, odor, with a, very, natural, violet, tonality, the, most, powerful, and pleasant isomer.
(R)-(+)-(E)-alpha-damascone, -
 odor, character, was, reminiscent of, rose, petals, with, apple, & fruitier, notes, than, (S)-(--)-(E)-alpha-
damascene, When used as a flavoring ingredient, (R)-(+) alpha-damascene, possesses also a somewhat woody, camphoraceous, dirty and musty taste. (S)-(−) alpha-damascene, is floral, reminiscent of rose petals and characterized by a more pronounced and fresher floral note, possessing more, a green and slightly winy notes, without presenting the "cork" tone and, and the typical green, apple, note of the, racemic mixture, or of the, (R)-(−)-enantiomer. When used as a flavoring ingredient, (S)-(−) alpha-damascene develops, a floral note. Moreover, it is reminiscent of tea, especially with regard to its herbal character.

(R)-gamma-damascene, - Liquidice, damascene-like, camphoraceous, inferior to, the, (S)-enantiomer.

(S)-gamma-damascene, - Nice, damascene, character, camphoraceous.

Methyl (R)-alpha-cyclogeranate, a, precious, flowery, fruity, damascene-like fragrance.

Methyl (S)-alpha-cyclogeranate, - characterised, by a, green, metallic, minty, camphoraceous note.

Methyl (R)-gamma-cyclogeranate, - more, common, than, (S)-enantiomer, camphoraceous, corky, cellar.

Methyl (S)-gamma-cyclogeranate, - aromatic, damascene-like, thujone, fruity.

(+)-Methyl (1R,2S)-delta-cyclogeranate.

Perfumers, have also noticed, some differences, between the, two, enantiomers, although, the odor, of both, enantiomers, is clearly damascene-like, and, in, the, same, trend, described, the, fragrance of, the, (1R,2S)-(−)-enantiomer, is, stronger, than, the, (1S,2R)-(−)-enantiomer, which, in, the, other, hand, is, more, aromatic.

(-)-Methyl (1S,2R)-delta-cyclogeranate, - less, strong, and, more, aromatic, than, the, (1R,2S)-(−)-enantiomer.

Ethyl (R)-gamma-cyclogeranate, - less, fruity, aromatic, rosemary, less, powerful, than, the, (S)-enantiomer.

Ethyl (S)-gamma-cyclogeranate, - aromatic, fruity, damascene-like.

Allyl (R)-gamma-cyclogeranate, - more, green, less, blackcurrant, less, floral, weaker, than, the, (S)-enantiomer.

Allyl (S)-gamma-cyclogeranate, - green, floral, blackcurrant, aromatic, fruity, pleasant.

(1R,6S)-(−)-ethyl tetrahydrosaffranate, - clean, and, sweet, floral.

(1S,6R)-(−)-ethyl tetrahydrosaffranate, - dirty, and, heavy, fatty, floral.

(1R,6S)-(−)-1,6-dihydromdamascene, - ripe, fruity, odor, with, fresh, rosy, note.

(1S,6R)-(−)-1,6-dihydromdamascene, - slightly, camphoraceous, fruity, odor, like, beta-damascene.

(1R,6S)-(−)-1',2,3,6'-tetrahydromdamascene, - heavy, fruity.

(1S,6R)-(−)-1',2,3,6'-tetrahydromdamascene, - fruity, odor, with, slight, peach, note.

(1S,6S)-(−)-1,6-dihydronone, - very, strong, violet, leaf, odor, like, alpha-ionone, (Yamamoto, et, al.), aromatic, carvone, woody, humus, powder, ionone, myrrh, violet, strong, (Chapuis, & Branchi).

(1R,6R)-(−)-1,6-dihydronone, - weak, woody, odor, with, chemical, note, (Yamamoto, et, al.), woody, ionone, leather, camphor, weak, (Chapuis, & Branchi).

(R)-(−)-Dihydro-alpha-ionone, - Floral, violet-type, odor, with, slightly, fruity, aspects. Also, possesses a, woody, side, but, less, pronounced, than, in, dihydro-beta-ionone.

(S)-(−)-Dihydro-alpha-ionone, - Exhibits, a, floral, orris-type, odor, with, woody, aspects, and, a, distinct, honey, note.

(R)-(−)-Dihydro-gamma-ionone, - Emanates, a, fatty, earthy, odor, with, floral, orris-type, nuances.

(S)-(−)-Dihydro-gamma-ionone, - Fatty, floral, odor, less, orris-type, than, the, other, compounds, of, the, dihydro, series. An, animalic, undertone, is, also, present.

(1R,6S)-(−)-Tetrahydroionone, - Woody, powder, amber, ionone.

(1S,6R)-(−)-Tetrahydroionone, - Woody, cedar, powder.

(-)-dihydro-beta-ionol, - excellent, retaining, properties, and, a, fine, floral, musky, type, fragrance, accompanied, with, a, high-class, feeling.

(+)-dihydro-beta-ionol, - excellent, retaining, properties, and, a, fine, floral, amber, fragrance, accompanied, with, a, high-class, feeling.

(1R,6S)-(−)-tetrahydroionol, - diffusive, amber, odor, with, slightly, floral, orris-type, and, earthy, note.

(1S,6R)-(−)-tetrahydroionol, - faint, vetiver-like, woody, odor.

(1R,6S)-(−)-1-(2',2',6'-Trimethylcyclohexyl)-pentan-3-one, - Woody, iron, weak.

(1S,6R)-(−)-1-(2',2',6'-Trimethylcyclohexyl)-pentan-3-one, - Amber, woody, saffron.

(1S,6S)-(−)-1-(2',2',6'-Trimethylcyclohexyl)-pent-1-en-3-one, - Oily.
(1'R,6'R)-(−)-1-(2',2',6'-Trimethylcyclohexyl)-pent-1-en-3-one,−, Saffron, woody, floral
(1S,6'S)-(−)-1-(2',2',6'-Trimethylcyclohexyl)-hex-1-en-3-one,−, Liquor, quince, violet, woody, powdery
(1'R,6'R)-(−)-1-(2',2',6'-Trimethylcyclohexyl)-hex-1-en-3-one,−, Woody, dry
(1'R,3'S,6'S)-(−)-1-(2',2',3',6'-Tetramethylcyclohexyl)-pentan-3-one,−, Woody, weak, irone
(1'S,3'R,6'R)-(−)-1-(2',2',3',6'-Tetramethylcyclohexyl)-pentan-3-one,−, Woody
(1'S,3'R,6'S)-(−)-1-(2',2',3',6'-Tetramethylcyclohexyl)-pent-1-en-3-one,−, Woody, Orris, powdery, myrrh, balsamic
(1'R,3'R,6'R)-(−)-1-(2',2',3',6'-Tetramethylcyclohexyl)-pent-1-en-3-one,−, Woody
(1'R,6'S)-(−)-1-(2',2',6'-Trimethylcyclohexyl)-pentan-3-ol,−, very, diffusive, sharp, amber, odor, with, slight, orrisy, camphoraceous, side, note
(1'R,6'R)-(−)-1-(2',2',6'-Trimethylcyclohexyl)-pentan-3-ol,−, faint, vetiver-like, woody, odor, with, slight, amber, and, moldy, note
(1'R,3'S,6'S)-(−)-3'-methyl-norlimbanol,−, woody-amber, odor, of, extraordinary, intensity,−, together, with, a, slight, transpiration, side, note
(1'S,3'R,6'R)-(−)-3'-methyl-norlimbanol,−, a, much, weaker, odor, albeit, of, similar, character, to, the, (+)-
(1'R,3'S,6'S)-isomer
(1'R,6'R)-(−)-5-methyl-norlimbanol,−, woody, notes
(1'S,6'R)-(−)-5-methyl-norlimbanol,−, woody, notes, but, much, weaker, than, the, (+)-(1'R,6'S)-isomer
(1'R,3'R,6'S)-(−)-norlimbanol,−, very, weak, and, devoid, of, animal, character
(1'S,3'S,6'R)-(−)-norlimbanol,−, elegant, woody-amber, note, similar, to, the, (1'R,3'S,6'S)-isomer, but, much, weaker
(1'R,3'S,6'S)-(−)-norlimbanol,−, strong, very, elegant, woody-amber, note, strongest, of, 4, trans, isomers
(1'S,3'R,6'R)-(−)-norlimbanol,−, very, weak, and, devoid, of, animal, character
(1'S,3'R,6'S)-(−)-4'-dihydroirone,−, iris-irone, note, with, a, very, warm, balsamic-myrrh, woody, character, The, violet-iris, character, is, more, pronounced, than, in, (1'R,3'R,6'R)-(−)-
enantiomer, or, the, racemate, and, the, odor, note, is, even, stronger
(1'R,3'R,6'R)-(−)-4'-dihydroirone,−, Woody, powdery, incense.
The, description, given, for, racemate, is,−, iris-violet, note, powder, balsamic, reminiscent, of, myrrh, woody, exceptional, strength, and, tenacity, odor
(1'R,3'S,6'S)-(−)-Tetrahydroirone,−, Woody, powdery, ambergris
(1'S,3'R,6'R)-(−)-Tetrahydroirone,−, Unpleasant
(1'S,5'R)-(−)-cis-alpha-irone,−, iris, sweet, irone, odor, woody, ionone, floral, fruity, (Galfrey, et, al., by, GC, sniffing), violet, like, with, woody, met
hydroionone, undertones, (Brenna, et, al.,)
(1'R,5'S)-(−)-cis-alpha-irone,−, odorless, (Galfrey, et, al., by, GC, sniffing), in, contrast, Inoue, et, al., indicate, the, (-)-
cis-alpha-irone, fragrance, is, superior, to, its, enantiomer, Brenna, et, al., describe, it, as, slightly, stronger, with, a, distinct, 'orris-butter', character
(1'S,5'S)-(−)-trans-alpha-irone,−, floral, fresh, &, fruity, irone, and, ionone, type, honey, sweet, chamomile, effect, violet, odor, is, weak, (Galfrey, et, al.,
by, GC, sniffing), Brenna, et, al., describe, it, as, the, weakest, of, the, alpha-isomers
(1'R,5'R)-(−)-trans-alpha-irone,−, iris, sweet, irone, character, dry, odor, (Galfrey, et, al., by, GC, sniffing), Brenna, et, al., describe, it, as, showing, a, "weak, violet, wood, red, berry, character, Neither, (+)-, nor, (−)-trans-alpha-
irone, possesses, the, characteristic, 'orris', odor"
(1'S,5'R)-(−)-cis-gamma-irone,−, iris, sweet, woody, ionone, dry, floral, (Galfrey, et, al., by, GC, sniffing), Inoue, et, al., indicate, the, (-)-
cis-gamma-irone, fragrance, is, Floral, green, weak, Brenna, et, al., describe, it, as, showing, a, floral, fatty, sweet, and, woody, odor, character, an, ionone, type, odor, with, slightly, sweet, aspects
(1'R,5'S)-(−)-cis-gamma-irone,−, odorless, (Galfrey, et, al.), in, contrast, Inoue, et, al., indicate, the, (-)-cis-gamma-
irone, fragrance, is, superior, to, its, enantiomer, with, Floral, sweet, ionone-like, notes, Brenna, et, al., describe, it, as, showing, a, "beta-ionone-type, odor, of, warm, floral-
woody, tonality, Green, aspects, are, present, too, It, shows, some, fruity, nuances, reminiscent, of, pineapples, The, odor
is, linear, and, it, can, be, considered, a, dry-down, note"
(1S,5S)-(−)-trans-gamma-ironne, iris and floral note, ionone, like, trans-alpha-ironne, (Galfry, et al., by GC, sniffing); Brenna, et al., describe it as, not, very, powerful, but, it possesses, a, soft, 'orris-butter' type, of, odor

(1R,5R)-(−)-trans-gamma-ironne,
weak, burnt, smell, metallic, chemical, (Galfry, et al., by GC, sniffing); Brenna, et al., describe it as, very, weak, of, a, woody, odor, tonality

(5R)-(−)-beta-ironne,
iris family, anis, liquorice, green, (Galfry, et al., by GC, sniffing); Brenna, et al., describe it as, possessing a, beta-ionone type, of, warm, floral-
woody, tonality, with, green, and, anisic, aspects, The odor, is, linear, and, the tenacity, of, the, note, is, good, It, can, be, considered, a, dry-down, note

(5S)-(−)-beta-ironne,
poor, weakly, iris, (Galfry, et al., by GC, sniffing); Brenna, et al., describe it as, having a, woody, odor, with, a, distinct,
honey, note, that, is, quite, sweet, Besides, it, shows, floral, ionone-
type, facets, and, a, fruity, tonality, but, also, an, unpleasant, smoky, character, It, belongs, to, the, beta-ionone-
type, family, without, being, very, close, to, beta-ionone

(1S,6R)-(−)-trans-2,2,6-trimethyl-cyclohexyl, methyl, ketone, - pleasant, mint-like, camphor-like,
 fragrance, that, is, extremely, sharp, strongly, dispersing, and, characteristic

(1R,6S)-(−)-trans-2,2,6-trimethyl-cyclohexyl, methyl, ketone, -
characteristic, marine, ozone, and, white, floral, fragrance, in, which, the, mint-like, and, camphor-
like, fragrance, is, weaker, resulting, in, a, softer, aroma, overall

(1R,2S,6'S)-(−)-1-(2',2',6'-trimethylcyclohexyloxyl)-2-pentanol, -
much, more, powerful, than, the, three, other, possible, optically, active, isomers, its odor, possesses, a, top, note, of, the,
amber, type, which, is, particularly, strong, accompanied, by, a, woody, note, less, pronounced, than, in, the, other, isomer
s, its fragrance, is, also, characterised, by, its, dryness, and, an, original, costus, note, which, is, lacking, in, the, odor, of, th

(1R,2R,5'R)-(−)-1-(2',2',6'-trimethylcyclohexyloxyl)-2-pentanol, -
odoriferous, notes, of, the, woody, type, but, much, less, powerful, than, the, (1'R,2'S,6'S)-(−)-isomer

(1R,2S,3'S,6'S)-(−)-1-(2',2',3',6'-tetramethylcyclohexyloxyl)-2-pentanol, -
the best, odorant, ingredient, of, the, series, possessing, a, fragrance, which, is, much, more, intense, and, long-
lasting, than, that, of, the, other, optically, active, isomers, its fragrance, is, extremely, intense, woody, fragrance, also, has, an, amber-
dented, dry, very, natural, character

(1S,2S,3R,6'R)-(−)-1-(2',2',3',6'-tetramethylcyclohexyloxyl)-2-pentanol, -
less, intense, and, shorter, lasting, fragrance, than, the, (1'R,2'S,3'S,6'S)-(−)-isomer

(+)-(1R,2S,3'R,6'S)-(−)-1-(2',2',3',6'-tetramethylcyclohexyloxyl)-pentan-2-ol, -
possesses, a, fragrance, which, is, much, more, intense, and, long-
lasting, than, that, of, the, other, possible, optically, active, isomers, its fragrance, also, has, an, amber-
dented, dry, very, natural, character

(-)(1S,2R,3'R,6'R)-(−)-1-(2',2',3',6'-tetramethylcyclohexyloxyl)-pentan-2-ol, -
much, weaker, than, the, (+)

(1R,2S,3'S,6'S)-(−)-1-(2',2',3',6'-trimethylcyclohexyl)-hexan-3-one, - ionone, woody

(2S,8aR)-3,4-Dihydro-3-oxocean, -
in the mixture, of, 2S, 8aS, (see, below), and, 2S, 8aR, isomers, (2S, 8aS, : 2S, 8aR, ratio, of, 15:85), a, camphoraceous, note, domin-
ated

(2R,8aS)-3,4-Dihydro-3-oxocean, -
in the mixture, of, 2R, 8aS, (see, below), and, 2R, 8aR, isomers, (2R, 8aR, : 2R, 8aS, ratio, of, 15:85), a, weak, tobacco, note, was, detectable

(2S,8aS)-3,4-Dihydro-3-oxocean, -
in the mixture, of, 2S, 8aS, and, 2S, 8aR, isomers, (2S, 8aS, : 2S, 8aR, ratio, of, 15:85), a, camphoraceous, note, domin-
ated

(2R,8aR)-3,4-Dihydro-3-oxocean, -
in the mixture, of, 2R, 8aR, and, 2R, 8aS, isomers, (2R, 8aR, : 2R, 8aS, ratio, of, 15:85), a, weak, tobacco, note, was, dete-
stable

(-)(2R,5'R)-Theaspirane, - weak, camphoraceous notation
Acyclics, (Alcohols,, Esters,, Acids,, Aldehydes)

(R)-(+)–2-methylbutanol,-fermented, fatty
(S)-(+)–2-methylbutanol,-etheral, fresh
(S)-(+)–2-methylbutanol,-pungent, fresh, fruity, (Boelens, et al.), peculiar, to, burnt, cocoa, and, coffee, like, in, high, concentrations, pungent, (Bartschat, et al.)
(R)-(+)–2-methylbutanol,-pungent, caprylic, (Boelens, et al.), peculiar, to, burnt, cocoa, and, coffee, like, (Bartschat, et al.)
(3S)-3-methylpentanal,-intensive, green, fresh, in, high, concentrations, sweet(y), & faint, fruity, in, low, concentrations,-slightly, pungent, odor
(3R)-3-methylpentanal,-no, fragrance, impression, at, >2.5, ppm, in, air
(4S)-4-methylhexanal,-no, fragrance, impression, at, >0.25, ppm, in, air
(4R)-4-methylhexanal,-intensive, flowery, warm, with, a, green, & fresh, note
(S)-(+)–2-methylbutanoic, acid,-fruity, sweet
(R)-(+)–2-methylbutanoic, acid,-cheesy, sweaty
(S)-(+)–4-methylhexanoic, acid,-caprylic, slightly, fatty
(R)-(+)–4-methylhexanoic, acid,-stronger, than, (S)-(+)–isomer, more, fatty
(4S)-4-methyloctanoic, acid,-muttony, goaty, fresher, than, the, (R)-enantiomer
(4R)-4-methyloctanoic, acid,-muttony, goaty, fusty
(S)-(+)–4-ethyloctanoic, acid,-goaty, reminiscent, of, fresh, goat’s milk, cheese
(R)-(+)–4-ethyloctanoic, acid,-fusty, goaty-muttony
(4S)-4-methylnonanoic, acid,-more, intensive, the, the, (R)-enantiomer, reminiscent, of, mutton, & goat
(4R)-4-methylnonanoic, acid,-weak, sweaty
Methyl, (S)-(+)–2-methylbutanoate,-fruity, apple-like
Methyl, (R)-(+)–2-methylbutanoate,-fruity, dairy
Ethyl, (S)-(+)–2-methylbutanoate,-fresh, fruity, apple-like
Ethyl, (R)-(+)–2-methylbutanoate,-fruity, caprylic
Ethyl, (S)-(+)–3-methyl-2-oxo-pentanoate,-a, typical, walnut, note, accompanied, by, a, walnut-husk, pungent, etheral, slightly, fruity, odor
Ethyl, (R)-(+)–3-methyl-2-oxo-pentanoate,-typical, walnut, note, but, its, odor, is, more, pungent, more, dry, less, powerful, and, does, not, possess, the, fruity-apple, note, present, in, the, (S)-isomer
(+)–Ethyl,(2R)-2-(1,1-dimethylpropoxy)propanoate,-a, comutation, of, the, chamomile, type, This, note, is, particularly, distinct, in, the, odor, of, the, ethyl, (R)-2-(1,1-dimethylpropoxy)propanoate, whose, fruity, note, is, also, very, strong.
(-)–Ethyl,(2S)-2-(1,1-dimethylpropoxy)propanoate,-a, more, spicy, note, which, also, comprises, a, chamomile, type, under, note, and, other, notes, reminiscent, of, ethyl, 2-acetyl-4-methyl-4-pentanone, the, wine, lees, linalool, and, also, coriander
(S)-2-pentylacetate,-fruity, apple, plum, metallic
(R)-2-pentylacetate,-fruity, Muscat, green, metallic, chemical
(S)-2-hexylacetate,-sweaty, sour, fruity, plum, nectarine
(R)-2-hexylacetate,-sour, fruity, cherry, plum, strawberry
(S)-(+)–2-heptylacetate,-Mushroom, earthy, wild, berry, (Nozaki, et al.); also, described, as, fruity, (Boelens, et al.)
(R)-(+)–2-heptylacetate,-Green, fatty, banana, methyl, ketone, (Nozaki, et al.); also, described, as, penetrating, sweaty, (Boelens, et al.)
S)-2-octylacetate,-Methyl, ketone, fruity, plum, dusty
(R)-2-octylacetate,-Methyl, ketone, fatty, burnt, boiled, vegetable
(S)-(+)-2-pentyl hexanoate,- pleasant, fruity
(R)-(-)-2-pentyl hexanoate,- flower,like
(S)-3-Acetoxyheptane,- exhibits a, rosy, fresh, agrest, scent.
(R)-3-Acetoxyheptane,- exhibits a, green, fruity, pear, scent.
(R)-4-(2-methyl-1-pentenyloxy)butyrate,- a, fruity, apricot, scent, with, rosy, bay, leaf, and, butyric, notes.
(S)-4-(2-methyl-1-pentenyloxy)butyrate,- a, prune, scent, with, mossy, camphorous, and, butyric, notes.
(S)-2-pentanol,- Heavy, wild, berry, ripe, dusty, astringent
(R)-2-pentanol,- Light, seedy, sharp
(S)-2-hexanol,- Mushroom, green, ripe, berry, astringent, metallic
(R)-2-hexanol,- Mushroom, dusty, oily
(S)-2-heptanol,- Mushroom, oily, fatty, blue, cheese, mouldy
(R)-2-heptanol,- Fruity, sweet, oily, fatty
(S)-3-Hydroxyheptane,- exhibits a, lavender, medicinal, scent
(R)-3-Hydroxyheptane,- exhibits an, earthy, mushroom, scent.
(S)-2-octanol,- Mushroom, oily, fatty, creamy, grape
(R)-2-octanol,- Creamy, cucumber, fatty, sour
(S)-1-hexen-3-ol,- Metallic, green, earthy
(R)-1-hexen-3-ol,- Top, impact, acid, meat, stronger, than, the, (S)-enantiomer
(S)-1-hepten-3-ol,- Fruity, earthy
(R)-1-hepten-3-ol,- Chemical, diffusible, green
(S)-1-oceten-3-ol,- moldy, grassy, artifical, also, described, as, herbaceous, green, musty
(R)-1-oceten-3-ol,- fruity, genuine, mushroom-like, also, described, as, intensive, mushroom, note, fruity, soft
(S)-1-nonen-3-ol,- Heavy, metallic, aldehydic
(R)-1-nonen-3-ol,- Mushroom, cheesy, fruity
(S)-1-decen-3-ol,- Metallic, oily, waxy, earthy
(R)-1-decen-3-ol,- Heavy, aldehydic, lactone
(2S)-3-mercapto-2-methylpropan-1-ol,- Weaker, than, the, (2R)-enantiomer, Although, both, of, the, enantiomers, are, characterized, by, the, same, broth, and, sweat, odour, they, have, very, different, odour, strength, and, thresholds.
(2R)-3-mercapto-2-methylpropan-1-ol,- Stronger, than, than, the, (2S)-enantiomer, Although, both, of, the, enantiomers, are, characterized, by, the, same, broth, and, sweat, odour, they, have, very, different, odour, strength, and, thresholds.
(3R)-3-mercaptohexan-1-ol,- In, dilution, the, (R)-enantiomer, is, distinctly, weaker, showing, only, sulfury, and, herbaceous, odor, impressions, (description of, Werkhoff, et al.)
(3S)-3-mercaptohexan-1-ol,- In, dilution, possesses, interesting, exotic, and, tropical, fruit, notes, (description of, Werkhoff, et al.), Werkhoff, et al, described, the, 3-mercaptohexanois, as, fruity, juicy, tropical, fruits, grapefruit, blackcurrant, buccan, mango, guava
(3R)-3-acetylidiohexanol,- fruity, grapefruit, sulfurous
(3S)-3-acetylidiohexanol,- sulfurous, roasted, rubberlike
(3R)-3-mercaptohexenal,- sulfurous, rubberlike
(3S)-3-mercaptohexenal,- green, citrus, peal, fruity
(3R)-3-acetylidiohexenal,- sulfurous, roasted, citrus, peel
(3S)-3-acetylidiohexenal,- fruity, sweet, grapefruit
(S)-3-(3-(methylthio)-hexan-1-ol,- spice-like
(R)-3-(3-(methylthio)-hexan-1-ol,- tropical, fruity, exotic
(3R)-3-mercaptohexylacetate,- In, dilution, possesses, attractive, tropical, fruity, notes, (for, the, (3R)-3-mercaptohexylacetate, and, (3R)-3-mercaptohexylacetate, butanoate).
(3S)-3-mercaptohexylacetate, (for, the, (3S)-3-mercaptohexylacetate, and, (3S)-3-mercaptohexylacetate, butanoate).
(3R)-3-mercaptohexylbutanoate,- In, dilution, possesses, attractive, tropical, fruity, notes, (for, the, (3R)-3-mercaptohexylbutanoate, and, (3R)-3-mercaptohexylacetate, (for, the, (3S)-3-mercaptohexylacetate, and, (3S)-3-mercaptohexylacetate, butanoate).
(3S)-3-mercaptobenzylbutanoate,

\textit{In dilution possesses insignificant sulfur, herbaceous, and oniony characteristics, for the (3R)-3-
mercaptobenzylbutanoate and (3R)-3-mercaptobenzylacetate, (description of Werkhoff., et., al.)}

(R)-(+) 2-ethylhexanoic, acid-, herbaceous, earthy

(S)-(+) 2-ethylhexanoic acid-, sweet, herbaceous, faint, musty

(2R,3S)-3-mercapto-2-methyl-pentane-1-ol, -broth-like, sweaty, leek-like

(2S,3R)-3-mercapto-2-methyl-pentane-1-ol, -broth-like, sweaty, leek-like

(2R,3S)-3-mercapto-2-methyl-pentane-1-ol, -broth-like, sweaty, leek-like

(2R,3R)-3-mercapto-2-methyl-pentane-1-ol, -broth-like, sweaty, leek-like

(R)-(+) 2,5,6-trimethyl-2-heptanol,-

odor, typical of white flowers, reminiscent of linalool, with a slight connotation of terpineol, and a lilac, and fruit

y note

(S)-(+) 2,5,6-trimethyl-2-heptanol, -more, floral, and citrus-

like, showing a note, reminiscent of dimethylctanol, -a, soap, and a, slight, aldehyde, connotation

(4S,5S)-(+) epoxy-(E)-2-decenal, -At 0.02, ppb, in, water, -no, smell, -no, taste, (weakest, enantiomer)

(4R,5R)-(+) epoxy-(E)-2-decenal, -At 0.02, ppb, in, water, -faint, smell, mild, metallic, taste, (strongest, enantiomer)

(+)-(E,R)-Filbertone, [(+),(E,R)-5-methyl-2-heptan-4-one], -

hazelnut, soft, butter, chocolate, metallic, weaker, impact, (at, 25, ppb, in, water)

(+)-(E,S)-Filbertone, [(+),(E,S)-5-methyl-2-heptan-4-one], -

hazelnut, metallic, fatty, pydine, stronger, impact, (at, 25, ppb, in, water)

**Lactones**

(R)-(+) 4-methylbutan-4-olide,- faint, sweet

(S)-(+) 4-methylbutan-4-olide,- faint

(R)-(+) 4-ethylbutan-4-olide,- faint, sweet, coconut, hatty, herbaceous, hay, note

(S)-(+) 4-ethylbutan-4-olide,- sweet, creamy, coconut, woody, aspects

(R)-(+) 4-propylbutan-4-olide,- sweet, spicy, herbaceous, hay, note, coumarin-like

(S)-(+) 4-propylbutan-4-olide,- fatty, coconut, note, fruity, sweet, aspects

(R)-(+) 4-butylbutan-4-olide,- spicy-green, coconut, note, almond, note

(S)-(+) 4-butylbutan-4-olide,- fatty, coconut, less, intense, than, (R)-isomer

(R)-(+) 4-pentylbutan-4-olide,- strong, sweet, soft, coconut, fatty, milky, aspect

(S)-(+) 4-pentylbutan-4-olide,- fatty, moldy, weak, coconut, less, intense, than, (R)-isomer

(R)-(+) 4-hexylbutan-4-olide,- strong, fatty, sweet, fruity, note, somewhat, coconut, caramel

(S)-(+) 4-hexylbutan-4-olide,- soft, sweet, coconut, note, fruity, fatty, aspects

(R)-(+) 4-heptylbutan-4-olide,- strong, fatty, sweet, peach, bloomy, aspects

(S)-(+) 4-heptylbutan-4-olide,- fatty, sweet, aldehyde, note

(R)-(+) 4-octylbutan-4-olide,- strong, fruity, sweet, bloomy, aldehyde, woody, aspects

(S)-(+) 4-octylbutan-4-olide,- fatty, fruity, milky, note, less, intense, than, (R)-isomer

(3S,4S)-(+) cis-3,4-Dimethylbutanoleide,- Faint, fatty, nutty, molds, odor

(3R,4R)-(+) cis-3,4-Dimethylbutanoleide,- Faint, sweet, hay, note

(3R,4S)-(+) trans-3,4-Dimethylbutanoleide,- Faint, spicy, fatty, fruity, note

(3S,4R)-(+) trans-3,4-Dimethylbutanoleide,- Faint, fatty, spicy, note

(3R,4S)-(+) 4-butyl-3-methylbutan-4-olide,- strong, coconut, note, reminiscent, of, celery

(3S,4R)-(+) 4-butyl-3-methylbutan-4-olide,- piquant, celery, note, faint, coconut, note, green, walnut, note

(3R,4R)-(+) 4-butyl-3-methylbutan-4-olide,- sweet, woody, bright, fresh, coconut, note

(3S,4S)-(+) 4-butyl-3-methylbutan-4-olide,- faint, coconut, note, faint, musty, earthy, reminiscent, of, hay

(R)-(+) 5-pentylpentan-5-olide,- sweet, fruity, milk, note

(S)-(+) 5-pentylpentan-5-olide,- sweet, fruity, peach, note, fatty, butter-like

(R)-(+) 5-hexylpentan-5-olide,- Fruity, sweet, creamy

(S)-(+) 5-hexylpentan-5-olide,- Fruity, sweet, milky

(R)-(+) 5-heptylpentan-5-olide,- Fruity, sweet, apricot
(S)-(−)-5-heptylpentan-5-olide, *Fruity*, sweet
(4S,5S)-(−)-cis-4-methyl-5-decanolide, or (4S,5S)-(−)-cis-Aragisins, lactone, -
reminiscent of, certain aspects of, the smell of, the flower of, the tuberosa, (Polianthes tuberosa), and, gardenia, varieties, and, on the other hand, is reminiscent of, caramel, condensed milk, and, coconut, especially, coconut milk
(4R,5R)-(−)-cis-4-methyl-5-decanolide, or (4R,5R)-(−)-cis-Aragisins, lactone, -reminiscent of, delta-decalactone and, coconut, and, with a fragrance, intensity, much lower, than, the, (4S,5S)-isomer
(4S,5R)-trans-4-methyl-5-decanolide, or (4S,5R)-trans-aragisins, lactone, -reminiscent of, delta-decalactone and, cocos, with similar, intensity, to, the, cis-(4R,5R)-enantiomer, and, higher, than, the, trans-(4R,5S)-enantiomer
(4R,5S)-trans-4-methyl-5-decanolide, or (4R,5S)-trans-aragisins, lactone, -
showed, slightly, lactonic, fragrance, with, the, lowest, fragrance, intensity, of, all, the, stereoisomers
(S)-(−)-(Z)-7-gamma-decenolactone, -creamy, milky, soft, caramel, fruity, gamma-decalactone-like, weakly, peach-like
(R)-(−)-(Z)-7-gamma-decenolactone, -racemate-like, fruity, intensive, peach-like, coconut, distinctly, stronger, than, (S)-(−)-, antipode
(S)-(−)-(Z)-7-delta-decenolactone, -fatty, creamy, less, intensive, than, racemate
(R)-(−)-(Z)-7-delta-decenolactone, -milky, coconut, fruity, less, intensive, than, racemate, distinctly, stronger, than, (S)-(−)-, antipode
(4R)-gamma-hexadecanolate, -green, grassy
(4S)-gamma-Octadecanolactone, -mushroom-like, odor, hay-like, odor, pungent
(4R)-gamma-Octadecanolactone, -mushroom-like, odor, hay-like, odor
(4S)-gamma-Decanolate, -sweet, fruity
(4R)-gamma-Decanolate, -fruity
(4S)-delta-Hexadecanolactone, -maggie-like, odor, sulfurous, burnt
(4R)-delta-Hexadecanolactone, -maggie-like, odor, spicy, burnt
(4S)-delta-Octadecanolactone, -mushroom-like, odor, grassy, hay-like, odor, sulfurous
(4R)-delta-Octadecanolactone, -mushroom-like, odor, grassy, green
(4S)-delta-decanolate, -sweet, fruity
(4R)-delta-Decanolate, -green, slightly, sweet, slightly, fruity
(3R)-Butylphthalide, -Herbaceous, celery-like, odor, This, enantiomer, shows, a, significantly, higher, GC, odor, threshold, value, than, does, the, (3S)-enantiomer.
(3S)-Butylphthalide, -Herbaceous, celery-like, odor, This, enantiomer, shows, a, significantly, lower, GC, odor, threshold, value, than, does, the, (3R)-enantiomer.
(3S,3aS,7aR)-3-Butylhexahydrophthalide, -sweet, and, sickly
(3R,3aR,7aS)-3-Butylhexahydrophthalide, -odorless
(+)-(3R,3aS,6R,7aR)-perhydro-3,6-dimethyl-2-benz[b]furanone, -
very, powerful, coumarinic, odor, notes, sweet, with, a, caramel, type, character
(-)-(3R,3aR,6S,7aS)-perhydro-3,6-dimethyl-2-benz[b]furanone, (87% pure), -
Odor: butyric, rancid, coumarinic, lactonic, sulfur, powerful.
(-)-(3R,3aS,6R,7aS)-perhydro-3,6-dimethyl-2-benz[b]furanone, (98% pure), -
coumarinic, lactonic, cold, tobacco, side
(+)-(3R,3aR,6S,7aR)-perhydro-3,6-dimethyl-2-benz[b]furanone, -coumarinic, hay, earthy, lactonic
(-)-(3R,3aR,6S,7aR)-perhydro-3,6-dimethyl-2-benz[b]furanone, -coumarinic, flowy, hay, sulfur, rubbery
(+)-(3S,3aS,6S,7aR)-Perhydro-3,6-dimethyl-2-benz[b]furanone, -description, not, given
(+)-(3S,3aS,6R,7aR)-perhydro-3,6-dimethyl-2-benz[b]furanone, -
tonka, beans, hay, flowy, type, characters, are, best, represented, whose, coumarinic, character, is, more, marked, in, the, bottom, note, than, in, the, top, note, and, is, accompanied, of, a, metallic, side
(-)-(3R,3aS,6S,7aS)-perhydro-3,6-dimethyl-2-benz[b]furanone, -description, not, given
(-)-(3S,3aS,6R,7aS)-perhydro-3,6-dimethyl-2-benz[b]furanone, -
coumarinic, flowy, hay, vaguely, sulphury, odor.
(+)-(3S,3aS,6S,7aR)-perhydro-3,6-dimethyl-2-benz[b]furanone, -description, not, given
(+)-(3S,3aS,6R,7aR)-perhydro-6-methyl-3-methylene-2-benz[b]furanone, -
coumarinic, lactonic, tonka, daffodil, very, powerful, perhydro-6-methyl-3-methylene-2-benz[b]furanone. possesses, a, very, powerful, odor, of, the, coumarinic, fat, lactonic, type, with, a balsamic, bottom, n
ote reminiscent of the odor of daffodil. This is an odor note, which is very close to that of coumarin, and which is best represented in (+)-(3aS,6R,7aR)-perhydro-6-methyl-3-methylene-2-benzo[b]furanone, (-)-(3aR,6S,7aS)-
perhydro-6-methyl-3-methylene-2-benzo[b]furanone, -Not available
(3aS,6R,7aR)-perhydro-6-methyl-3-methylene-2-benzo[b]furanone, -coumarinic, lactonic, tonka
(3aR,6S,7aR)-perhydro-6-methyl-3-methylene-2-benzo[b]furanone, -not available
(+)-(6R)-3(RS)-3,6-dimethyl-4,5,6,7-tetrahydro-1-benzofuran-2(3H)-one, -it develops a phenolic/coumarin-like odor, making it a useful alternative to coumarin. It also has a completely original, minty, odoriferous note, much appreciated by perfumers
(-)-(6S)-3(RS)-3,6-dimethyl-4,5,6,7-tetrahydro-1-benzofuran-2(3H)-one, -not available
(-)-(3aS,6R,7aS)-perhydro-3,5,6-trimethyl-2-benzo[b]furanone, -lactonic, fruity, coumarinic
(+)-(3aR,6S,7aR)-perhydro-3,5,6-trimethyl-2-benzo[b]furanone, -not available
[3aS,3aR,7aR]-Wine, lactone, -intense, sweet and coconut-like, (coumarinic), this is the naturally occurring enantiomer
[3aS,3aR,7aS]-Wine, lactone, -description not available
[3aS,3aR,7aR]-Wine, lactone, -description not available
[3aS,3aR,7aS]-Wine, lactone, -description not available
[3aS,3aR,7aR]-Wine, lactone, -description not available
[3aS,5aS,7aR]-Wine, lactone, -description not available
[3aR,5R,7aR]-5-isopropenyl-7a-methylhexahydro-1-benzofuran-2(3H)-one, -moderately intense, agreeable, herbaceous odor, with lupine, flower and parsley, root, notes
[3aS,5S,7aS]-5-isopropenyl-7a-methylhexahydro-1-benzofuran-2(3H)-one, -faint, mushroomy, and moldy, with a floral, note.
Sesquiterpenoid, & Diterpenoid Related Odorants
(-)-(4S)-patchouliol, -like patchouli oil
(+)-(4S)-patchouliol, -not like patchouli oil, woody, with underlying green notes
[2S,5R]-(-)-thaispirane, -highly attractive, intense, fresh-fruity
[2S,5R]-(+)-thaispirane, -naphthalene-like
[2S,5R]-(+)-thaispirane, -weak, camphoraceous note
[2S,5S]-(-)-thaispirane, -fresh, camphoraceous note
[2S,4aS]-(-)-alpha-ambrinol, -powerful amber note, with a natural, somewhat musky and animal, character
[2S,4aR]-(+)-alpha-ambrinol, -exhibits a strongly dry, earthy, musty, tonal note, reminiscent of geosmin
(-)-Ambrox®, -moist, soft, creamy, persistent, warm, animalic, amber odor, with a velvety, effect
(+)-Ambrox®, -accentuated, woody, note, and lacks the strong animalic, warmth", of the, (-)-isomer
13-deoxyambrinolide, -pronounced, ambergris, aroma
ent-13-deoxyambrinolide, -odorless
(-)-3S,6R-Nootkatone, -strong, grapefruit odor, bitter, in taste
(-)-3S,6R-Nootkatone, -weak, woody, (vetiver, noe), no grapefruit character
(+)-(4R,4aS,6R,8aS)-Tetrahydro-nootkatone, -dusty-woody, -fresh, green, sour, spicy, herbal, slightly fruity, animal, erogenic
(-)-(4S,4aR,6S,8aR)-Tetrahydro-nootkatone, -dusty-woody, -spicy, -fresh, green, sour, slightly herbal, fruity, animal, erogenic
(+)-(4R,4aS)-(-)-alpha-vetivone, -some, grapefruit character, in combination, with its, strong, characteristic, woody, balsamic odor, also, has been, described as, floral-waxy-woody
(+)-(4S,4aR)-(-)-alpha-vetivone, -completely, lacks the, fruity, character, of, (+)-alpha-vetivone.
(+)-8-Dehydro-11, 12-dihydro-nootkatone, -On, an odor, rating, scale: -fresh, green, sour, dusty-woody, herbal,
spicy, slightly, animal, erogenic, fruity
(-)-8-Dehydro-11, 12-dihydro-nootkatone, -On, an odor, rating, scale: -dusty-woody, fresh, green, sour, herbal,
spicy, slightly animal, erogenic
(-)-(1aR,5S,6aR)-Tricyclodecane, -On, an odor, rating, scale: -dusty-woody, -fresh, green, sour, spicy, herbal, slightly, animal, erogenic
Chiral, partial structures of beta-Vetivone

(+)-(1α,5S,6αS)-Tricycloketone, -On an, odor, rating, scale; dusty-woody, spicy, slightly fresh, green, sour, herbal, animal, erogenous
R-(+)-(5)-nerolidol, -pleasant, woody, warm, musty
S-(2)-(E)-nerolidol, -slightly sweet, mild, soft, flowery, different, than, (S)-(Z)-isomer
R-(2)-(Z)-nerolidol, -intensive, flowery, sweet, fresh
S-(2)-(Z)-nerolidol, -woody, green-like, fresh, bark
(5R,10R)-(–)-beta-vetivone, -quinoline-like, fruity, (cassia, grapefruit), aroma, with, a woody, bynote, (the natural, enantiomer)
(5S,10S)+(–)-beta-vetivone, -unpleasant, cresolic, medicinal, note
(5R,10R)-(–)-6-demethyl-beta-vetivone, -a, sweet, coumarin-like, odor, with, a woody, note
(5S,10S)+(–)-6-demethyl-beta-vetivone, -a, woody, smell, with, a quinoline-like, bynote
(5S)-(–)-10-demethyl-beta-vetivone, -intense, cresolic
(5R)-(–)-10-demethyl-beta-vetivone, -intense, cresolic

(4S,5R)-(–)-3.5-Dimethyl-4-(4-methyl-pent-3-enyl)-cyclohex-2-ene-one, -fresh-woody, with, a low, intensity
(4R,5S)+(–)-3.5-Dimethyl-4-(4-methyl-pent-3-enyl)-cyclohex-2-ene-one, -
-an intense, but unpleasant phenolic, medicinal, scent
(4R,5R)-(–)-3.5-Dimethyl-4-(4-methyl-pent-3-enyl)-cyclohex-2-ene-one, -nearly odorless
(4S,5S)+(–)-3.5-Dimethyl-4-(4-methyl-pent-3-enyl)-cyclohex-2-ene-one, -nearly odorless
(4S,5R)-(–)-3.5-Dimethyl-4-(3-methyl-but-2-enyl)-cyclohex-2-ene-one, -weak, Cassia-like, scent, with, a sulfur-like, bynote
(4R,5S)+(–)-3.5-Dimethyl-4-(3-methyl-but-2-enyl)-cyclohex-2-ene-one, -balsamic, (myrrh-like), with, a woody, bynote
(4R,5R)-(–)-3.5-Dimethyl-4-(3-methyl-but-2-enyl)-cyclohex-2-ene-one, -weak, fresh-woody, and somewhat reminiscent, of, vetiveryl, acetate
(4S,5S)+(–)-3.5-Dimethyl-4-(3-methyl-but-2-enyl)-cyclohex-2-ene-one, -
-unpleasant, intense, phenolic, medicinal, scent
(2S,8αR)-3,4-Dihydro-3-oxoeculan, -
-In the mixture, of, 2S,8αS, (see, below), and, 2S,8αR, isomers,(2S,8αS, ; 2S,8αR, ratio, of, 15:85), a, camphoraceous, note, dominated, Using GC, sniffing, the, 3,4-dihydro-3-oxoeculans, exhibited, only, weak, odor, intensities
(2R,8αS)-3,4-Dihydro-3-oxoeculan, -
-In the mixture, of, 2R,8αR, (see, below), and, 2R,8αS, isomers,(2R,8αR, ; 2R,8αS, ratio, of, 15:85), a, weak, tobacco, note, was, detectable, Using GC, sniffing, the, 3,4-dihydro-3-oxoeculans, exhibited, only, weak, odor, intensities
(2S,8αS)-3,4-Dihydro-3-oxoeculan, -
-In the mixture, of, 2S,8αS, and, 2S,8αR, isomers,(2S,8αS, ; 2S,8αR, ratio, of, 15:85), a, camphoraceous, note, dominated, Using GC, sniffing, the, 3,4-dihydro-3-oxoeculans, exhibited, only, weak, odor, intensities
(2R,8αR)-3,4-Dihydro-3-oxoeculan, -
-In the mixture, of, 2R,8αR, and, 2R,8αS, isomers,(2R,8αR, ; 2R,8αS, ratio, of, 15:85), a, weak, tobacco, note, was, detectable, Using GC, sniffing, the, 3,4-dihydro-3-oxoeculans, exhibited, only, weak, odor, intensities
(+)-(2R,4αR,8αS)-Polywood®, -
-Odor, properties, described, as, exhibiting, a rich, voluminous, woody, note, with, a powdery, ionone-like, undertone.
(-)-(2S,4αS,8αR)-Polywood®, -Odor, properties, was, found, less, rich, than, (+)-(2R,4αR,8αS)-Polywood®, -still, woody, dry, and, amber-like.
(+)-(4αS,8αR)-5,5,8a-trimethyloctahydronaphthalen-2(1H)-one, -
-Odor, properties, described, as, strong, woody, amber-like, with, a distinct, note, of, damp, earth, cellar, geosmin.
(+)-(4αR,8αS)-5,5,8a-trimethyloctahydronaphthalen-2(1H)-one, -
-Odor, properties, was, found, woody, patchouli-like, and, less, strong, than, its, enantiomer.
(R,R)-Iso-beta-bisabolol, -very, strong, flowery, lilley-of-the-valley, like, and, very, pleasant, odor, -
-stronger, than, the, (1S)-1-{(1S)},(1R)-1-{(1S)}-OR, (1S)-1-{(1R)}-enantiomers
(S,S)-Iso-beta-bisabolol, -white, similar, not, as, strong, as, (1R)-1-{(1R)}-iso-beta-bisabolol
Steroid, Urine, Type, Odorants

(+)-androstene-3,17-dione, -strong, urine, odor
(-)-androstene-3,17-dione, -odorless
(-)-androst-4,16-dien-3-one, -odorless
(+)-androst-4,16-dien-3-one, -very, persistent, odor, of, urine, & sweat

Nature, Identical, Sandalwood, Odorants

(+)-(1'S,2'R,4'R)-(Z)-beta-santalol, -Typical, sandalwood, scent, identical, to, the, natural, product.
(+)-(1'R,2'S,4'S)-(Z)-beta-santalol, -No, scent, (odorless).
(+)-(1'S,2'R,4'R)-(E)-beta-santalol, -Scent, similar, to, (-)-(1'S,2'R,4'R)-(Z)-beta-santalol, but, less, intense.
(+)-(1'R,2'S,4'S)-(E)-beta-santalol, -No, scent, (odorless).

Sandalwood, Type, Odorants, from, Campholenic, aldehyde

(+)-(1'R)-4-(2',2',3'-trimethyl-3'-cyclopeten-1'-yl)-4-penten-1-ol, -
fragrance, further, possessing, an, aldehydic, note, reminiscent, of, citronella, citrus, spicy, recalling, the, odor, of, the, citronella, leaves, As, to, its, bottom, note, it, has, a, character, which, is, reminiscent, of, the, odor, of, 3-(4-tert-buty-1-
phenyl)-2-methylpropanol, but, with, an, even, greener, connotation, and, a, slightly, orangy, aspect

(+)-(1'S)-4-(2',2',3'-trimethyl-3'-cyclopeten-1'-yl)-4-penten-1-ol, -
a, more, metallic, and, aldehydic, odor, recalling, that, of, trans-4-
decenal, and, the, bottom, note, of, which, is, more, floral, and, even, stronger, in, the, aqueous, character, the, use, of, this, latter, compound, to, enhance, the, latter, odor, character, in, perfumed, compositions, and, articles, is, in, fact, preferred, to, that
of, its, (-)-(1'R)-enantiomer

(+)-(1'R)-2-methyl-4-(2',2',3'-trimethyl-3'-cyclopeten-1'-yl)-4-pentenonitrile, -a, woody-
citrus, fruity, and, slightly, fatty, odor, preferred, to, the, (+)-(1'S)-isomer

(+)-(1'S)-2-methyl-4-(2',2',3'-trimethyl-3'-cyclopeten-1'-yl)-4-pentenonitrile, -not, as, preferred, an, odor, as, the, (-)-(1'R)-isomer

(+)-(1'R,2'R)-2-methyl-4-(2',2',3'-trimethyl-3'-cyclopeten-1'-yl)-4-pentenonitrile, -
citrus, fruity, and, fresh, character, accompanied, by, a, sandalwood, bottom, character

(+)-(1'S,2'S)-2-methyl-4-(2',2',3'-trimethyl-3'-cyclopeten-1'-yl)-4-pentenonitrile, -
odor, not, described, other, than, to, say, the, (1'R,2'R)-isomers, are, preferred

(+)-(1'R,2'S)-2-methyl-4-(2',2',3'-trimethyl-3'-cyclopeten-1'-yl)-4-pentenonitrile, -
a, sandalwood, odor, wherein, the, desired, fruity-citrus, character, of, the, (-)-(1'R,2'R)-isomer, is, no, longer, present

(+)-(1'S,2'R)-2-methyl-4-(2',2',3'-trimethyl-3'-cyclopeten-1'-yl)-4-pentenonitrile, -
odor, not, described, other, than, to, say, the, (1'R,2'R)-isomers, are, preferred

(+)-(1'R,2'R)-2-methyl-4-(2',2',3'-trimethyl-3'-cyclopeten-1'-yl)-4-penten-1-ol, -
elegant, and, powerful, sandalwood, note, (preferred, of, the, four, isomers)

(+)-(1'S,2'S)-2-methyl-4-(2',2',3'-trimethyl-3'-cyclopeten-1'-yl)-4-penten-1-ol, -
odor, is, less, rich, in, the, precious, "santal, type", odor, character, present, in, the, (-)-(1'R,2'R)-, and, (-)-(1'R,2'S)-
isomers

(+)-(1'R,2'S)-2-methyl-4-(2',2',3'-trimethyl-3'-cyclopeten-1'-yl)-4-penten-1-ol, -
sandalwood, note, is, not, as, powerful, as, the, (-)-(1'R,2'R)-isomer, but, is, accompanied, of, a, more, marked, woody-
cedar, character

(+)-(1'S,2'R)-2-methyl-4-(2',2',3'-trimethyl-3'-cyclopeten-1'-yl)-4-penten-1-ol, -
odor, is, less, rich, in, the, precious, "santal, type", odor, character, present, in, the, (-)-(1'R,2'R)-, and, (-)-(1'R,2'S)-
isomers
(-)-(1R,E)-3,3-diethyl-5-(2',2',3',3'-trimethyl-3'-cyclopenten-1'-yl)-4-penten-2-ol,-
develops a sandalwood note, the character of which is strongly reminiscent of the typical, milky odor of sandalwood
(+)-(1S,E)-3,3-diethyl-5-(2',2',3'-trimethyl-3'-cyclopenten-1'-yl)-4-penten-2-ol,- drier, more woody,
cedar and less milky, than that of its, (–)-(1R,E)-isomer
(+)-(1S,2S,E)-3,3-diethyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol,-
develops a sandalwood note, of remarkable strength, wherein the typical, milky character is, represented at its best, a
nd accompanied by a slightly animal note; preferred of four, possible isomers
(-)-(1R,2R,E)-3,3-diethyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol,-
weakest and less characteristic sandalwood note, than any of the other, isomers
(+)-(1S,2R,E)-3,3-diethyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol,-
ranked in 3d place of 4, isomers for its sandalwood odor
(-)-(1S,2S,E)-3,3-diethyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol,-
weaker and less characteristic sandalwood note, than the, (+)-(1S,2S,E)-isomer, but superior to the, (+)-(1S,2R,E)-
or, (+)-(1R,2R,E)-isomers
(+)-(1R,E)-2-Methyl-4-(2',2',3'-trimethyl-cyclopenten-3-enyl)-but-2-en-1-ol,-
fresh and strong sandalwood, odor, associated, with green, trees
(+)-(1S,E)-2-Methyl-4-(2',2',3'-trimethyl-cyclopenten-3-enyl)-but-2-en-1-ol,-
dry and weak sandalwood, odor, with a milky and floral note
(+)-(1R,E)-2-Ethyl-4-(2',2',3'-trimethyl-cyclopenten-3-enyl)-but-2-en-1-ol,-
clean bright and strong sandalwood, odor, with richness and a woody note
(+)-(1S,E)-2-Ethyl-4-(2',2',3'-trimethyl-cyclopenten-3-enyl)-but-2-en-1-ol,-
milky sandalwood, odor, with a cedar character
(+)-(1R)-2-methyl-4-(2',2',3'-trimethyl-3'-cyclopenten-1'-yl)-4-penten-1-ol,-
possesses an unexpected odor, in view of the prior knowledge, regarding the odor, properties, of campholenic, aldehy
dye derivatives. It develops a woody-sandalwood, type, odor, note, slightly, aldehydic, which is more, reminiscent of the, cedar-
pine odor, connotation, than of, the sandalwood type, one, which note is combined, with a, distinct, marine, ozone, char
acter. The latter, is reinforced in the bottom, note, which is strongly, ozone-marine-
like, recalling the odor of, seaweeds. In addition, the odor of this compound has a, good, strength, and tenacity.
(+)-(1S)-2-methyl-4-(2',2',3'-trimethyl-3'-cyclopenten-1'-yl)-4-penten-1-ol,-
woody, sandalwood, aldehydic, faintly, aqueous
(+)-(1S)-1"R, 3"R, 3"S, 3"R-Javanol, - sandalwood, creamy, warm, strong
(+)-(1R,1"R, 2"R, 3"S, 5"S-Javanol, - lactonic, lily of the valley
(+)-(1R,1"S, 2"R, 3"R, 5"R-Javanol, - lactonic, with a, sandalwood aspect
(+)-(1S,1"R, 2"R, 3"S, 5"S-Javanol, - floral, rosy, milky, sandalwood
(+)-(1S,2"S)-5-(2,2-dimethyl-3'-methylene-1'-cyclohexyl)-3,3-dimethyl-4-penten-2-ol,-
Woody, sandal., sweet, note, reminiscent of the, odor, of, the bark, and milk, of, the, sandalwood, tree.
(+)-(1R,2"R)-5-(2',2'-dimethyl-3'-methylene-1'-cyclohexyl)-3,3-dimethyl-4-penten-2-ol,-
Sandalwood odor, but, distinctly, different, than the, (+)-(1S,2"S)-isomers

Other, Sandalwood, Odorants
(+)-(3R,3'R,1'S,2'S,4'S,6'S)-3,3-trans-3-isoamphylcyclohexanol, - Strong, diffusive, and sandalwood-
like odor, natural, sandalwood, odor, but, very, strong and keen
(+)-(3S,3'S,1'R,2'R,4'R,6'R)-3,3-trans-3-isoamphylcyclohexanol, - weak, moldy, and woody odor
(+)-(3S,3'S,1'S,2'R,4'R,6'S)-3'-erythro-3-trans-3-isoamphylcyclohexanol, -
sandalwood, like odor, without, moldy, feeling, and it is, sufficiently, diffusive
(+)-(3R,1'R,2'R,4'R,6'R)-3'-erythro-3-trans-3-isoamphylcyclohexanol, - strong, warm, sandalwood odor
(+)-(3S,3'R,6'R,8'R)-8'-tertbutylbicyclo[4,4,0]decan-3-ol,- Strong, Sandalwood odor
(+)-(3R,3'S,6'S,8'S)-8'-tertbutylbicyclo[4,4,0]decan-3-ol,- Odorless
(+)-(2S,3R,4R)-3-methyl-4-((1R,2R,6R,7R)-tricyclo[5.2.1.0^2,6]dec-4-en-8-yldene)butan-2-ol,-
very, strong, sandalwood, animalic
Musk Odorants

(4S,7R)-(+)−galaxolide,−powerful,musk,odor
(4R,7S)+−galaxolide,−weak,to,almost,odorless
(4R,7R)+−galaxolide,−weak,to,almost,odorless
(4S,7S)−galaxolide,−powerful,musk,odor
(R)-(−)−muscone,−rich,−powerful,−muskly,,very,nice,musky,,note,,rich,and,powerful,”
(S)+(−)−muscone,−poor,,weakly,musky
(12R,9Z)−Nirvanolide,−intense,musky,,fruity,,powdery,odor,with,lactic,nuances
(12S,9Z)−Nirvanolide,−odorless
(+)(11R)−11−methyl−12−dodecanolide,−
a,faint,musk,note,with,very,fresh,nuances,of,clary,sage,and,bergamot,is,accompanied,by,cedarwood,accents.,Only,a,slightly,earthy,musty,undertone,has,to,be,accounted.
(+)(11S)−11−methyl−12−dodecanolide,−The,smell,of,of,(S)−enantiomer,does,not,differ,much,in,its,sensory,qualities,however,its,is,of,weaker,intensity.
(12S)−(+)(12−methyl−13−tridecanolide,−animalic,musky,,camphoraceous
(12R)−(+)(12−methyl−13−tridecanolide,−sandalwood−like,musk,note
(12S,13R)−(+)(12−methyl−13−tetradecanolide,−animalic,,cedar,,wood,profile,with,camphoraceous,aspects,,devoid,of,musk,notes
(12R,13S)−(+)(12−methyl−13−tetradecanolide,−strong,,woody,odor,with,a,pronounced,musk,character
(12R)−(+)(12−methyl−9−oxa−14−tetradecanolide,−intense,,musk−
floral,,powdery,odor,,reminiscent,of,of,th,ni,tro,musk,ambrette,,with,additional,woody,,myrrh−type,factors
(12S)−(+)(12−methyl−9−oxa−14−tetradecanolide,−odorless
(+)(−)(S)−Muscolide,−weak,intensity,,but,possesses,a,very,pleasant,musk,note,,with,a,more,distinctive,erogenous−animalic,character.
(+)(−)(R)−muscolide,−slightly,erogenous,,animalic,,resembling,that,of,natural,musk,tincture.
(+)(−)(S)−Oxo−muscolide,−possesses,a,weak,musk,note,,without,animalic,character,,and,is,dominated,by,an,odour,reminiscent,of,ironed,linen.
(+)(−)(R)−Oxo−muscolide,−slightly,musky,and,sweet,,but,not,erogenous−animalic.
(2R,4S)−Oxomalolide,−an,amber,,fresh,sweet,,powdery,,slightly,musky,,dull,scents
(2R,4S)−Oxomalolide,−an,amber,,woody,,fresh,fragrance,of,Paris,mushrooms,,wood,glue,,slightly,pungent,scents
(+)(1R,4S)−Helvetolide,−Odor,properties:,musk,,ambrette,,pear,,The,fragrance,effect,imparted,by,the,above−
cited,preferred,compound,of,of,of,character,can,even,more,powerful,and,musky,when,said,compound,is,used,in,th
ese,form,of,one,of,its,optimally,active,iso,soms,,i.e.,(+)-(−)−Helvetolide
(−)(1S,4R)−Helvetolide,−Odor,properties:,nicely,musky,ambrette,,pear,,floral.
(1S,1R)−1−[(3′,3′−dimethyl−1′−cyclohexyl)−ethoxy,carbonyl]−methyl,propanoate,−
The,odor,properties,are,best,represented,in,of,of,of,configuration,(1S,1R),−which,renders,this,compound,a,choice,ingredient,of,of,character,This,compound,possesses,a,traditional,musky,character,reminiscent,of,that,of,Galaxolide(7),−dihydro−4,6,6,7,8,8−hexamethyl−6H−cyclopenta[9]−2−benzopyran,−and,confers,an,olfactive,impression,which,isa,that,of,a,sweet,and,natural,musky,odor,with,a,velvet,yness,texture,which,provides,rich,vs,olve.,There,is,also,found,a,light,ambrette,nuance,which,can,be,companioned,by,an,undernote,reminiscent,of,of,of,green,fruits.
(1R,1'S)-1-[(3',3'-dimethyl-1'-cyclohexyl)-ethoxycarbonyl]methyl,propanoate. This compound is less preferred than the (1S',1'R), enantiomer.

(3S)-(-)-3-Methyl-1,4-dioxacyclopentadecan-2-one, -musk, sweet-flowery, ambergris, erogenous, animalic, reminiscent of ambrette, musk, and nitromusk, weaker than the enantiomer, mixture.

(3R)-(+)-3-Methyl-1,4-dioxacyclopentadecan-2-one, -musk, sweet-flowery, ambergris, erogenous, animalic, reminiscent of ambrette, musk, and nitromusk, stronger than the (S)-(−)-enantiomer.

(3S)-(−)-3-Methyl-1,4-dioxacyclohexadecan-2-one, -musk, sweet-woody, ambergris, erogenous, animalic, reminiscent of ambrette, musk, and nitromusk, weaker than the enantiomer, mixture.

woody, ambergris, erogenous, animalic, reminiscent of ambrette, musk, and nitromusk, stronger than the (S)-(−)-enantiomer.
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Claims

1) A method for determining qualitatively or quantitatively one or more analytes present in a defined area of the body of a subject characterised by the following steps:
   
a) applying an adsorbent material to the defined area of the body of a subject,

   b) extracting the analyte from said area and removing the adsorbent material from the defined area of the body,

   c) desorbing the analyte from the adsorbent material, and detecting the analyte qualitatively or quantitatively.

2) The method according to claim 1 where steps a-d) are repeated at least once.

3) The method according to claim 1 or 2 where the area of the body is the oral cavity, the nasal cavity, the vagina, the anal cavity, hair, or another area of the skin.

4) The method according to any of claims 1 to 3 where a composition comprising the analyte or a precursor thereof is administered to a subject prior to the application of the adsorbent material.

5) The method according to claim 4 where the composition comprising the analyte or a precursor thereof is administered orally.

6) The method according to claim 1 for determining qualitatively or quantitatively one or more analytes after oral administration of a composition to a subject characterised by the following steps:

   a) oral administration of a composition comprising the analytes or a precursor thereof to a subject,

   b) contacting an adsorbent material with the saliva from said subject at a predefined starting point,

   c) extracting the analyte for a defined period from said saliva,

   d) desorbing the analyte from the adsorbent material,

   e) detecting the analyte qualitatively or quantitatively, and
f) optionally repeating steps a-e) or b-e) at least once where the starting point in b) differs and optionally the extraction period in c) may vary.

7) The method according to claims 5 or 6 where the adsorbent material is applied into the mouth, and extraction takes place within the mouth.

8) The method according to claims any of the preceding claims where the composition is selected from food, beverage, a matrix spiked with the analyte or a precursor, toothpaste, mouthwash, tobacco-ware or the smoke thereof.

9) The method according to claim 5 where the composition comprising the analyte or a precursor thereof is administered topically.

10) The method according to claim 5 or 9 where the adsorbent material is applied to the skin and extraction takes place at the surface of the skin.

11) The method according to claims 5 or 10 where the composition is selected from fragrances, deodorants, antiperspirants, skin care products, cleansing products, decorative cosmetic products, pharmaceutically active topical preparations, and mixtures thereof.

12) The method according to claim 5 where the composition comprising the analyte or a precursor thereof is administered nasally, anally, or vaginally.

13) The method according to claim 5 or 12 where the adsorbent material is applied to the nasal cavity, vagina, or anal cavity, respectively, and extraction takes place at the nasal cavity, vagina or anal cavity, respectively.

14) The method according to any of the preceding claims where the adsorbent material is selected from polydialkylsiloxanes, polyphenyleneoxides, divinylbenzene, polyacrylates, activated alumina, carbon black, carbon molecular sieves adsorbent resins, polyethylene glycols, diatomaceous earth based adsorbents and mixtures of two or more thereof.
15) The method according to any of the preceding claims where the adsorbent material is selected from polydialkylsiloxanes, Tenax®, divinylbenzene, carbowax/divinylbenzene, carboxen/PDMS, PDMS/divinylbenzene, carboxen/divinylbenzene, and polyacrylate.

16) The method according to any of the preceding claims where the adsorbent material is polydimethylsiloxane (PDMS).

17) The method according to any of the preceding claims where the analyte is selected from one or more of the following:
   - pharmaceutically active compounds,
   - cosmetically active compounds,
   - toxic compounds,
   - pheromones or hormones,
   - proteins, carbohydrates or fats present in food,
   - flavours,
   - compounds inducing a physical perception,
   or a degradation product of the above.

18) The method according to any of the preceding claims where the analyte is selected from proteins, carbohydrates, fats, tastants or other compounds inducing any kind of chemo- or physio-perception, types of compounds eliciting a trigeminal sensation in the in the nasal, oral or pharyngeal area, volatiles and odours.

19) The method according to any of the preceding claims where the desorption takes place via thermal desorption.

20) The method according to any of the preceding claims where the detection is performed by GC/olfactometry, GC/MS/olfactometry or high resolution gas chromatography (HRGC/O).

21) An adsorbent article suitable to be applied in the method according to any of claims 1 to 20 comprising:
   - a housing having at least three apertures located in a manner that they allow a free flow of a fluid into and out of the housing,
- an adsorbent material included within said housing.

22) The adsorbent article according to claim 21 comprising a porous capsule and an adsorbent material included therein.

23) The adsorbent article according to claim 21 or 22 wherein the housing is made of metal, glass, silicone, plastic, ceramics or porcelain.

24) The adsorbent article according to any of the preceding claims where the capsule is made of glass and is suitable to be introduced into the mouth.

25) The adsorbent article according to any of the preceding claims where the adsorbent material allows a thermal desorption of an analyte from same.

26) The adsorbent article according to any of the preceding claims where the adsorbent material allows an adsorption of an analyte by means of physisorption.

27) The adsorbent article according to any of the preceding claims where the housing has the form of a tube which has apertures distributed over the tube.

28) The adsorbent article according to claim 27 where the tube is releasably closed at both ends.

29) The adsorbent article according to any of the preceding claims where the housing has at least one flat surface with apertures distributed over said surface.

30) The adsorbent article according to any of the preceding claims where the housing is disposable.

31) A kit for an adsorbent article according to claims 21-30 comprising

- a housing having at least three apertures located in a manner that they allow a free flow of a fluid into and out of the housing,
- an adsorbent material to be included within said housing.
32) A patch comprising a layer of an adsorbent material and a support provided on said adsorbent material.

33) The patch according to claim 32 where the support comprises a backing layer having provided thereon a layer of an adhesive.

34) The patch according to claim 33 where the adsorbent material is attached to the backing layer via the adhesive layer.

35) The patch according to claims 33 or 34 where 5 to 40% of the surface of the adsorbent material is attached to the backing layer.

36) Beads, suitable to be used as adsorbent material according to claims 21-31, comprising PDMS, having a diameter from more than 0.05 mm to below 10 mm.

37) Use of an adsorbent article according to claims 21 to 30 for determining qualitatively or quantitatively one or more analytes.

38) The use according to claim 37 in solid phase extraction.

39) The use according to claim 37 in a method according to any of claims 1 to 20.

40) Use of a patch according to any of claims 32 to 35 for determining qualitatively or quantitatively one or more analytes.

41) The use according to claim 40 in a method according to any of claims 1 to 20.

42) Use of the method according to any of claims 1 to 20 for selecting relevant compounds for the manufacture of a composition to be administered to a subject.

43) Use of compounds which have been determined to be relevant according to the method as defined in any of claims 1 to 20 for the manufacture of a composition to be administered to a subject.
Figure 1.
Figure 2.
Figure 3.
Figure 4. a-c
d)

Figure 4. d
Figure 5.
Figure 6.
Figure 7.
Figure 8.
Figure 9.
A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 G01N1/40 G01N33/483 G01N1/34
//A61B10/00, A61F13/15

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 G01N A61B C12M

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic database consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, PAJ

C. DOCUMENTS CONSIDERED TO BE RELEVANT

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Date of the actual completion of the international search: 21 December 2004

Date of mailing of the international search report: 04/01/2005

Name and mailing address of the ISA

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