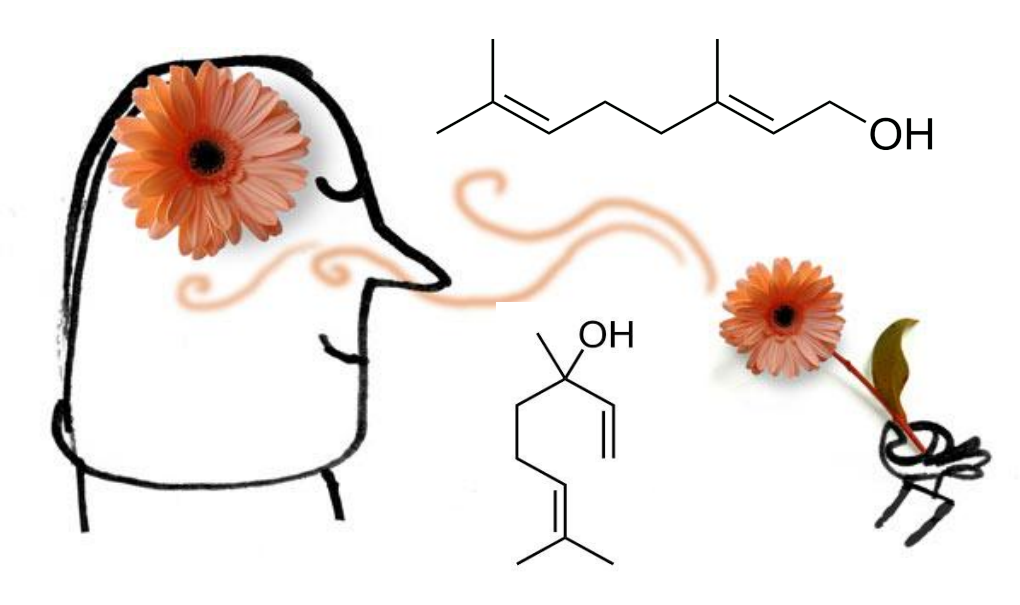
Flavour Chemistry

Science behind Taste and Smell for Agri-Business and the Food Industry



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Agribusiness in Schools National Conference, May 2024

University of Otago

ŌTĀKOU WHAKAIHU WAKA

Outline

- **What is Flavour Science**
  - Career opportunities
- **What is Flavour?**
  - How do we perceive flavour?
- **Flavour compounds and perception**
- **Research at Otago**

Outline

- What is Flavour Science?
- Career pathways

- Perception of Flavour
  - The senses
  - Flavour stimuli and Flavourings

- Research at Otago
  - Integrated capability
    - Through Chain “Farm to Fork” Approach
  - Hops and beer flavour
  - Extraction of flavour from waste streams

Samples to evaluate

- PROP
- Jelly beans – Retronasal demo
- Odour compounds to smell
- Bottles of citral – with and without Tastants

- Hops
- Rose samples and sniffing strips (pipette and tips)

Who am I?

- **Flavour scientist** (wait, what?)
- **My interests:**
  - **Understanding what makes food taste and smell the way it does…**
  - Analysis of aroma compounds
  - Hop chemistry and hop flavour in beer
  - Flavour generation during fermentation
  - Upcycling food waste
  - Flavours in vaping
    - Are they safe?
  - Sourdough, Smoked foods, milk, cheese, coffee and many more…

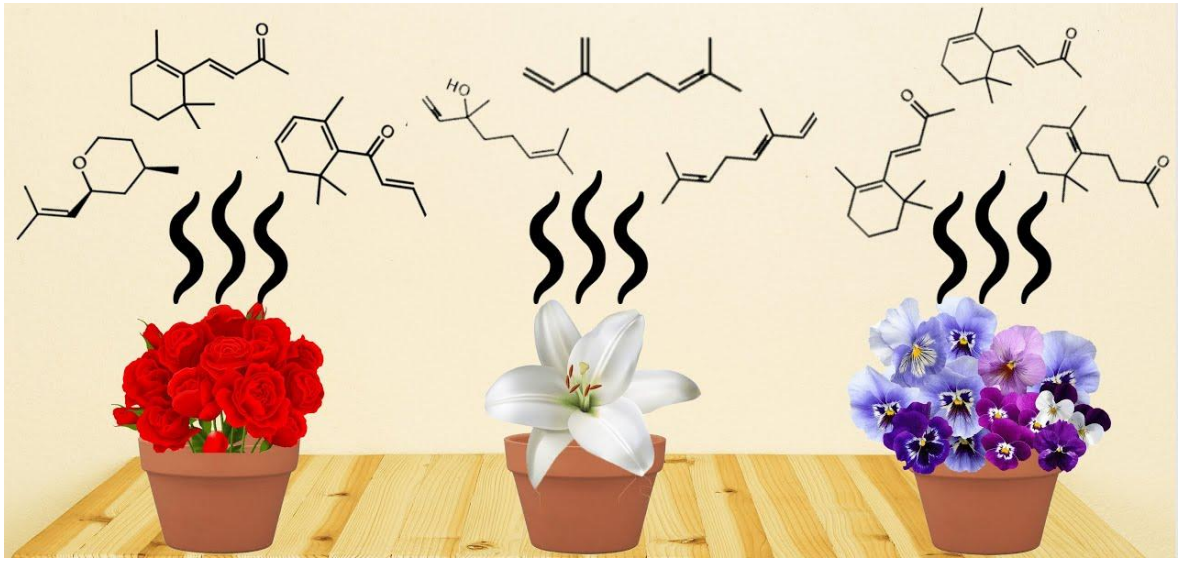
ODT article - ginger beer from waste
RNZ Brewing beer - from waste to taste

Objectives of this Workshop

"A taste of Flavour Chemistry"

- Appreciation of **Flavour Chemistry** and **Sensory Perception**.
- Importance and applications of **Flavour Science** for Agribusiness and the Food Industry.
  - Career pathways for Graduates
  - Engagement activities for Agribusiness students
- Research capability and projects at Otago

“What is responsible for that smell?”



Why do people perceive flavour differently?

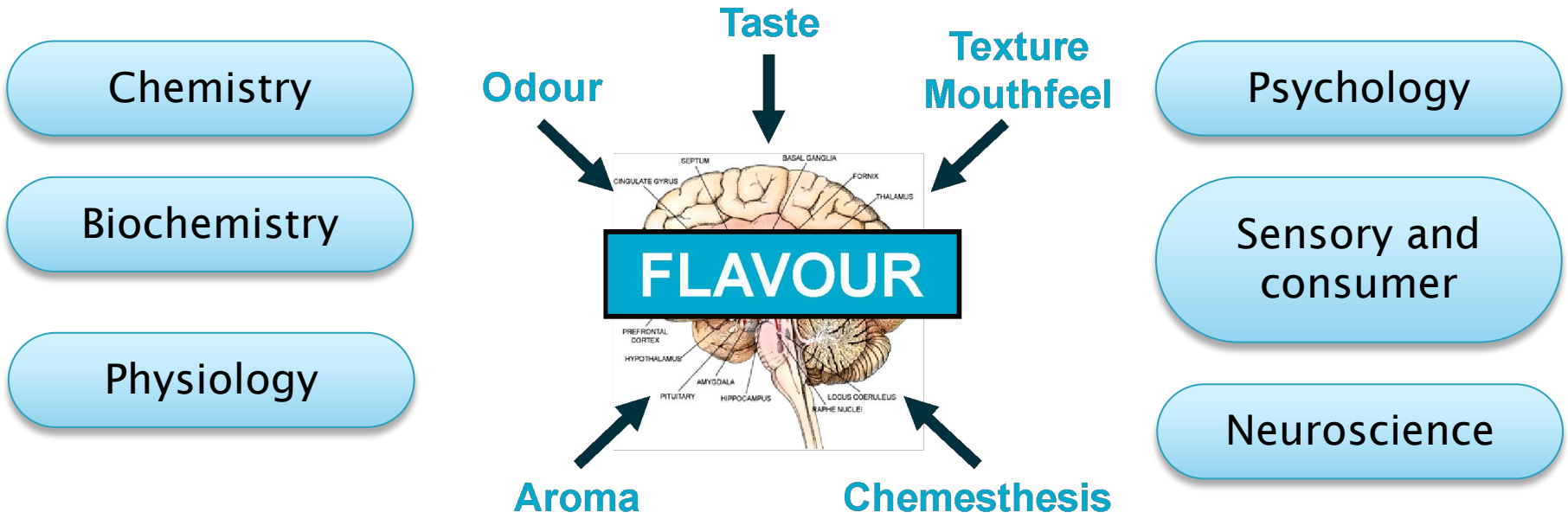
A food's success in the market, is dependent on the consumers perception.

If the package looks pretty, but what's inside does not taste good, **who's going to buy it?**

Sensory and Flavour science helps in all aspects during the creation and manufacture of products to ensure they best meet consumer demands.

What is Flavour Science?

- **Flavour Science seeks to:**
- Understand the physical and chemical factors that influence the sensory perception of flavour.



Sensory Science

- **Sensory Evaluation** is defined as:

"A scientific method used to evoke, measure, analyze and interpret those responses to products as perceived through the senses of sight, smell, touch, taste and hearing."

- ***Objectively*** measure the sensory properties of food and food products.

Career Opportunities

- World-wide Shortage of Food Science / Consumer Food Science graduates !
- Exciting and stimulating career prospects for Food Technologists
- Specialist flavour and sensory roles
  - Flavour companies
  - Food producers

- Flavour and Sensory expertise is also very important in product development and quality assurance roles.

The Flavour Industry

- Global sales estimated at **US$26.3 billion** (2017)
  - Top 11 companies control ~ 80% of the market

Rank	Company	2013 Sales US$ million	Market share
1	Givaudan	$5132.8	19.5%
2	Firmenich	$3668.4	13.9%
3	IFF	$3398.7	12.9%
4	Symrise	$2672.6	10.2%

Source: http://www.leffingwell.com/top_10.htm

What is Flavour?

Chemistr
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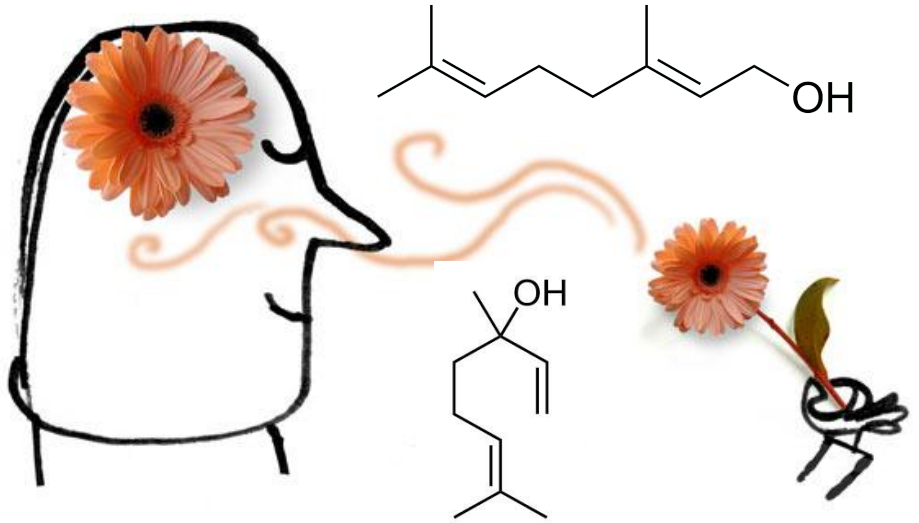
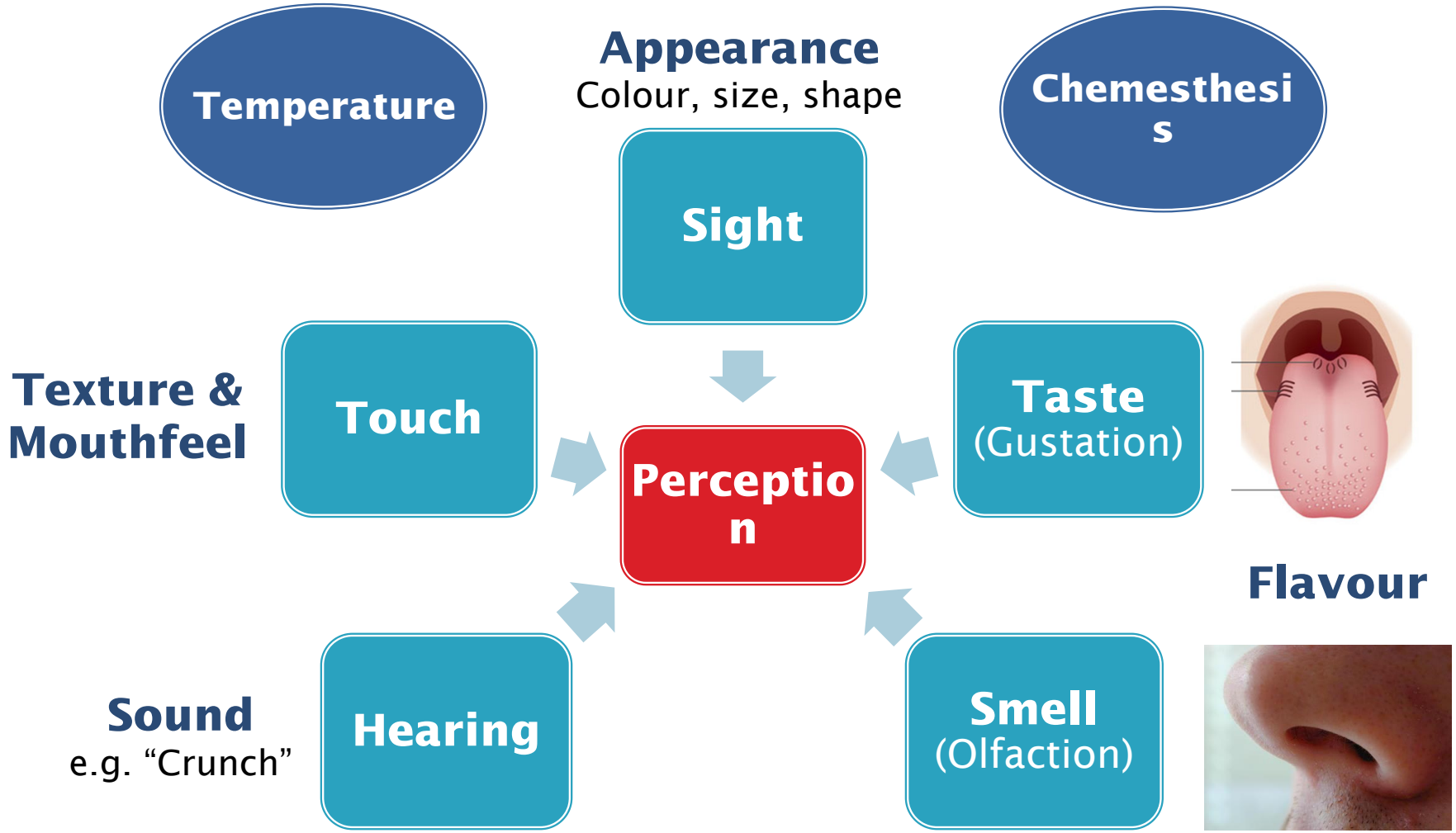


Perception

Chemistry ≠ Perception

The Senses


Temperature
Appearance
Colour, size, shape
Chemesthesis
Sight
Texture & Mouthfeel
Touch
Taste
(Gustation)
Perception
Flavour
Sound
e.g. “Crunch”
Hearing
Smell
(Olfaction)

The Senses

Temperature

Appearance
Colour, size, shape

Chemesthesis

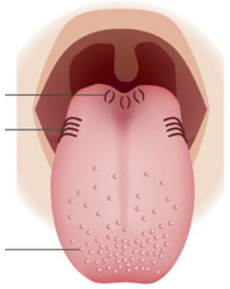
Sight

Texture & Mouthfeel

Touch

All of our senses (modalities) are **important when eating.**

Taste
(Gustation)



Flavour

Sound
e.g. “Crunch”

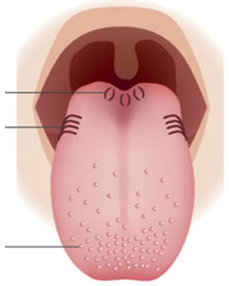
Hearing

Smell
(Olfaction)

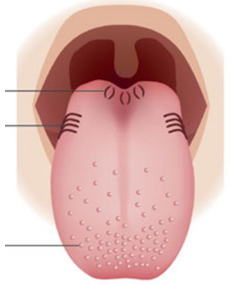
What is Flavour?

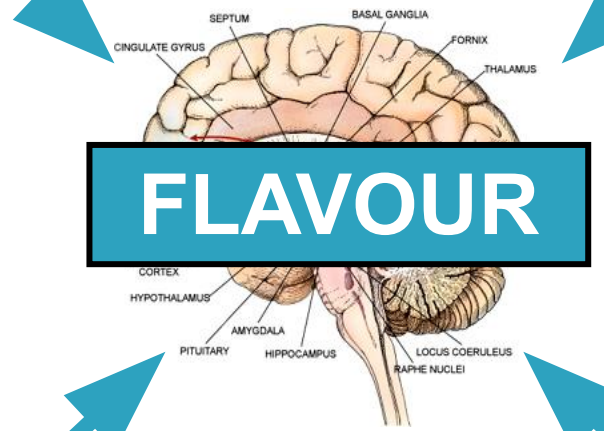
Odour
Olfaction via nose

Taste
Gustation on tongue



Texture
Mouthfeel
Mouth





Aroma
Olfaction via mouth

Extrinsic factors

Chemesthesis
Pungency, irritation, thermal sensations

What is Flavour Perception?

Flavour is a complex and integrated perception consisting of odour, aroma, taste, texture/mouthfeel and chemesthesis. *[1,2]*

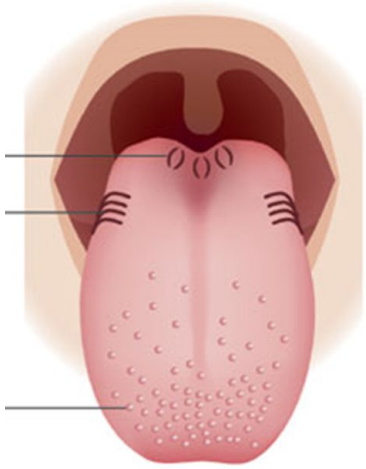
- **Flavour** often referred to as an ***emergent phenomenon*** or a ***psychological construct*****.** *[3,4]*
- Affected by biological and psychological factors of the individual and past experience.
- Affected by **extrinsic factors**: e.g. packaging, marketing and context effects.

Definition adapted from: [1] Lawless and Heymann (1998). Sensory Evaluation of Food. Springer, New York. [2] Dattatreya, Kamath and Bhat (2002). *Food Res. Int.* ***18***, 223-242.
[3] Delwiche (2012). *Physiol. & Behav., 107, 502-504.* [4] Prescott (1999). *Food Qual Pref 10, 349-356.*

Taste (Gustation)

- The sense of taste (**gustation**) detected by taste receptors on the tongue.
- There are **5 basic tastes:**
  - **Sweet**
  - **Sour**
  - **Salty**
  - **Bitter**
  - **Umami**

- **What foods are they associated with?**



How does Taste work?

The 'Taste Map'

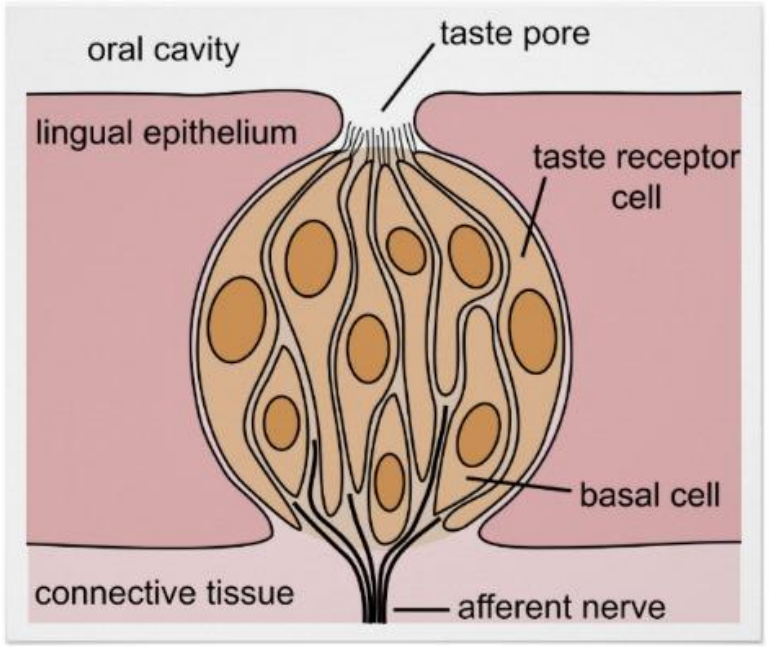
A MYTH!!

- **All taste qualities** can be elicited on **all regions** of the tongue that contain taste buds.
- However, some areas of the tongue may be more sensitive to specific tastes.
  - Tip of tongue most sensitive to sweet and bitter
  - Sourness most strongly perceived at rear

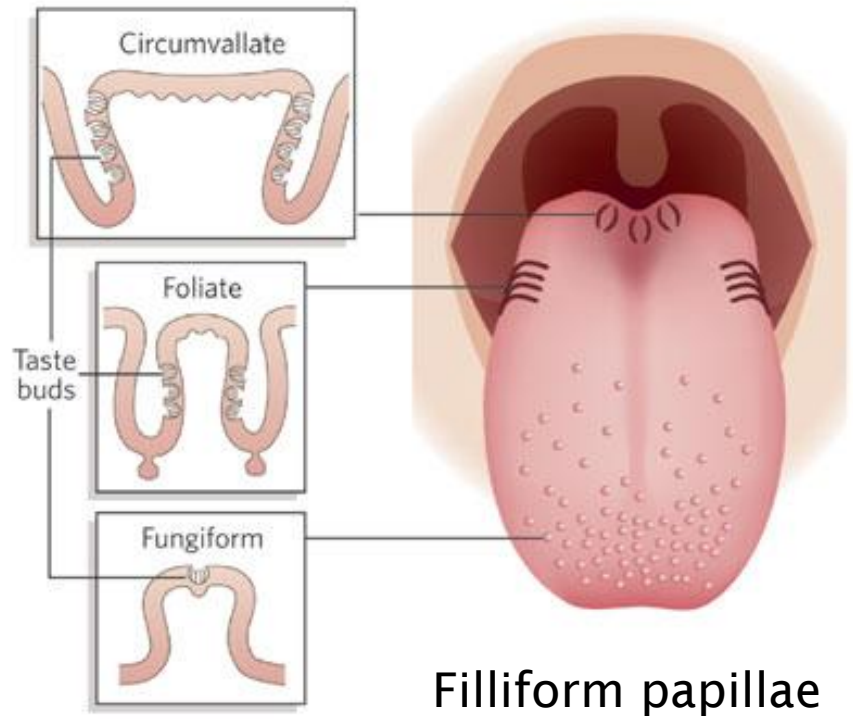
How does Taste work?

- Taste receptors located on ***Taste Receptor Cells (TRC)***
- ~30-50 TRCs make up each ***Taste Bud***
- ~10,000 taste buds in adults
- Taste buds are grouped within structures known as ***Papillae*** (4 types)

Taste Bud



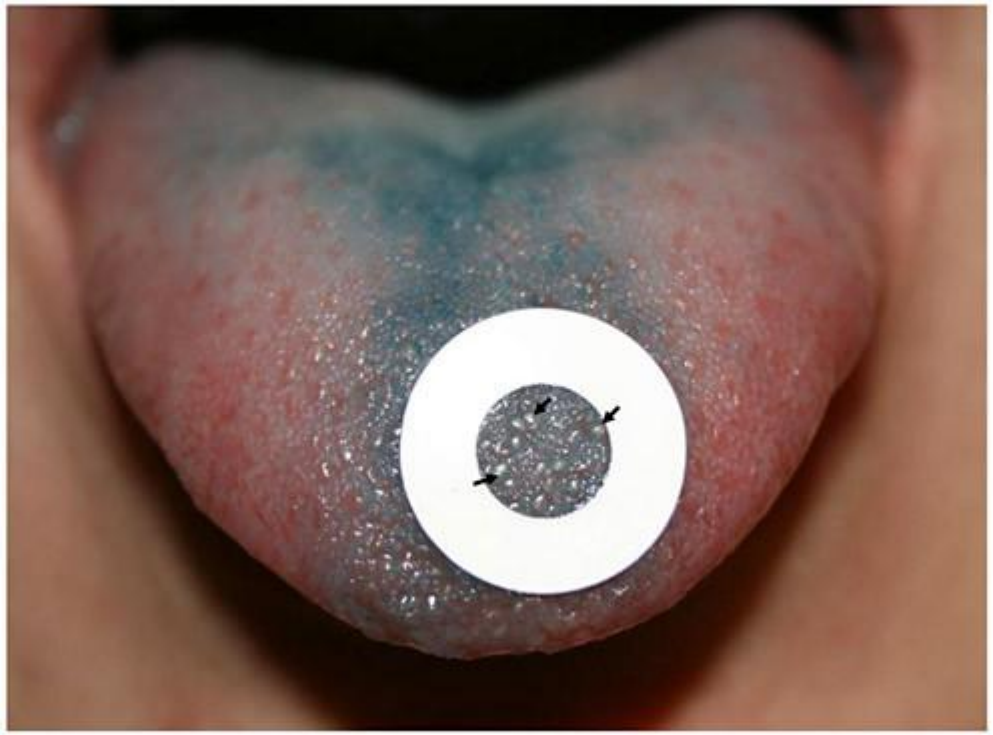
Papillae



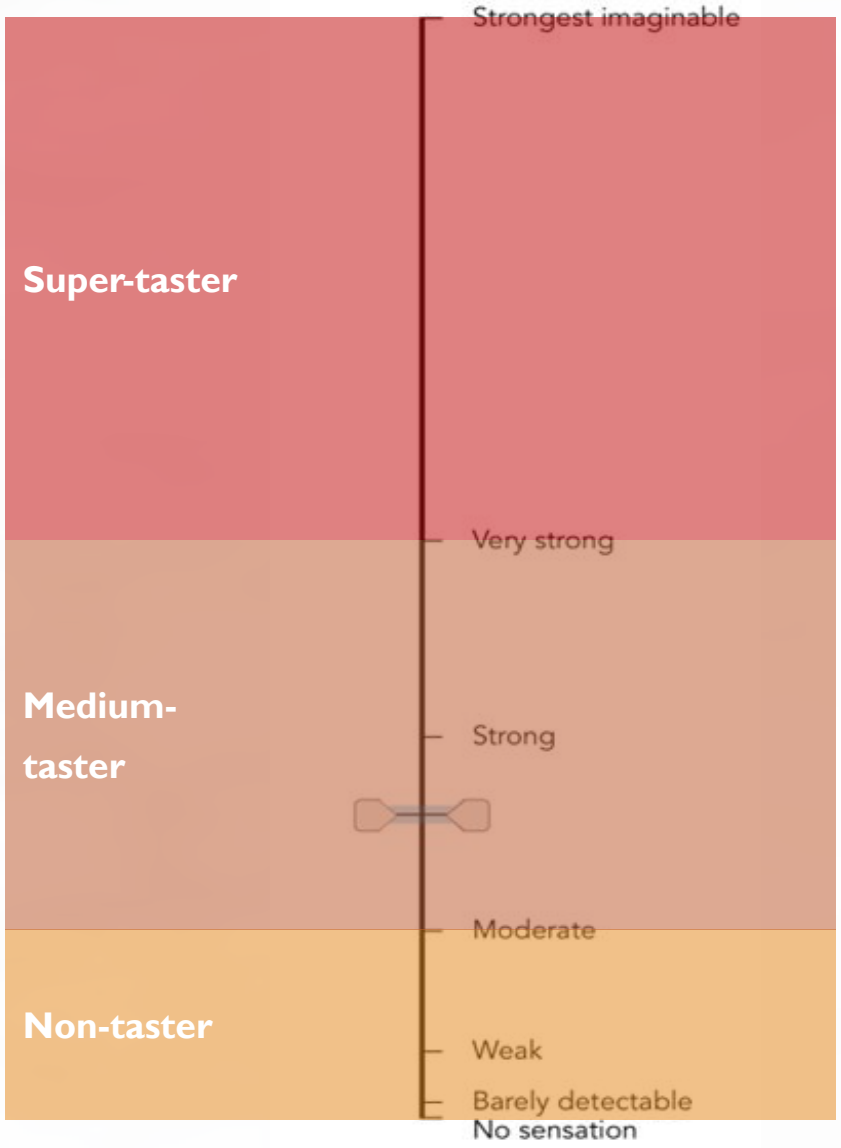
Filliform papillae
(no taste buds)

Taster Status

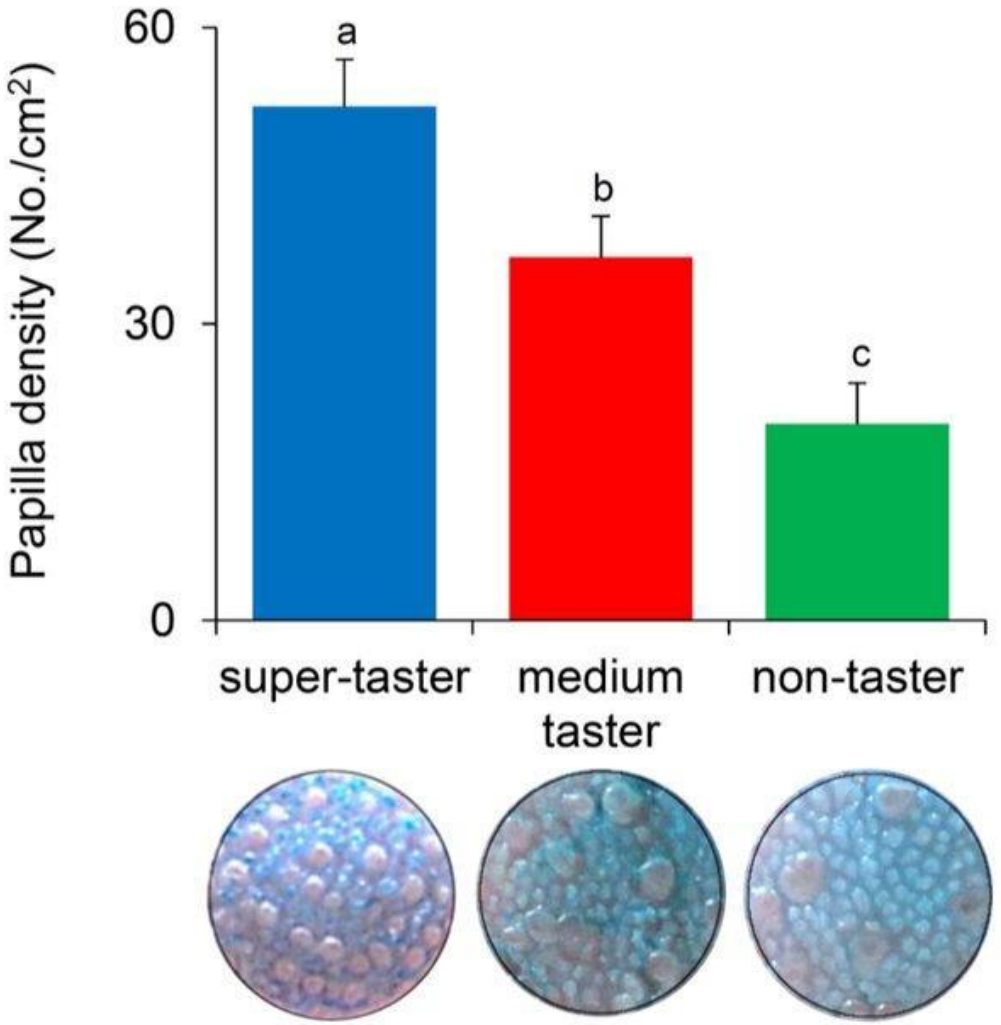
PROP (6-*n*-propylthiouracil)
Taste Pore Count



PROP Taster Status



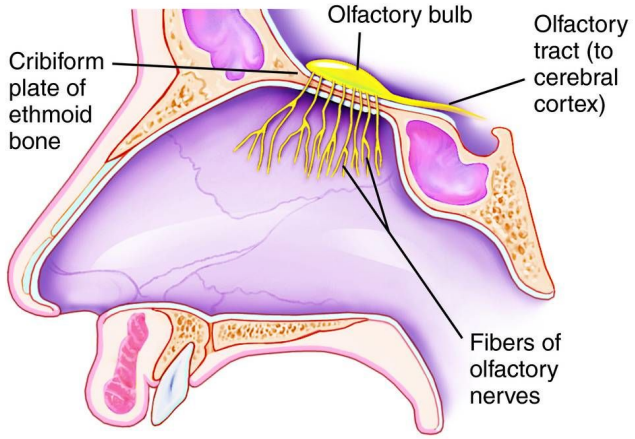
Papillae Count



Melis, M. et al. (2020). Electrophysiological responses from the human tongue to the six taste qualities and their relationships with PROP taster status. *Nutrients*. 12. 2017. https://doi.org/10.3390/nu12072017.

Smell (Olfaction)

- The sense of smell (**olfaction**) is detected by olfactory receptor cells (ORCs) located in the olfactory epithelium in the nasal cavity.



http://medical-dictionary.thefreedictionary.com
(11/02/2013)

- 6-8 million ORCs in the human nose
- 100-300 million ORCs in a dog's nose!!!
- As opposed to Taste, there are ***hundreds*** of odour and aroma qualities.

Smell (Olfaction)

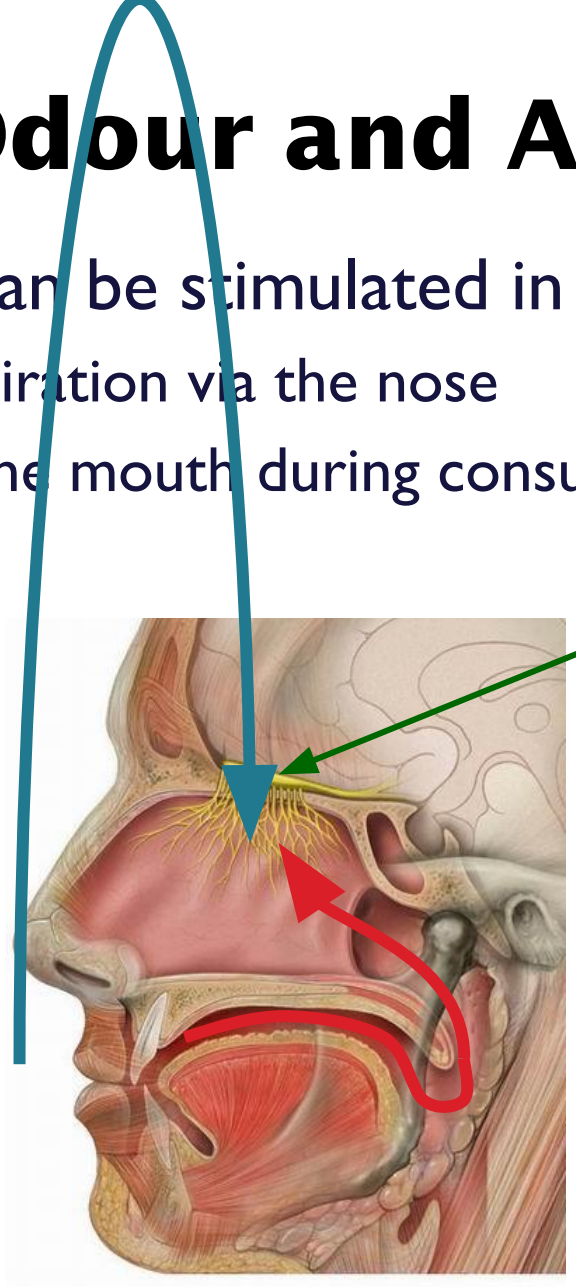
- What we usually call "**flavour**" is mediated by the sense of olfaction (smell) detected in the nose.
- Responsible for the wide diversity of **flavour characters**.
  - Distinguishes the identity of flavour character
    - E.g. Strawberry vs Raspberry
  - Food flavour is made up of hundreds of aroma compounds
    - >200 compounds in strawberry
    - >1000 compounds in coffee

Skittles…

- **Take a Skittle but DON'T eat it yet**
- Hold your nose firmly between your fingers
- Place the Jelly Bean into your mouth and chew (keep hold of your nose)
- What do you **taste**?
- Release your nose and **breath out**.
- What is the **flavour**?

Olfaction – Odour and Aroma

- Sense of olfaction can be stimulated in two ways:
  - **Orthonasal** – inspiration via the nose
  - **Retronasal** – via the mouth during consumption



Olfactory receptors

Odour
(via nose)

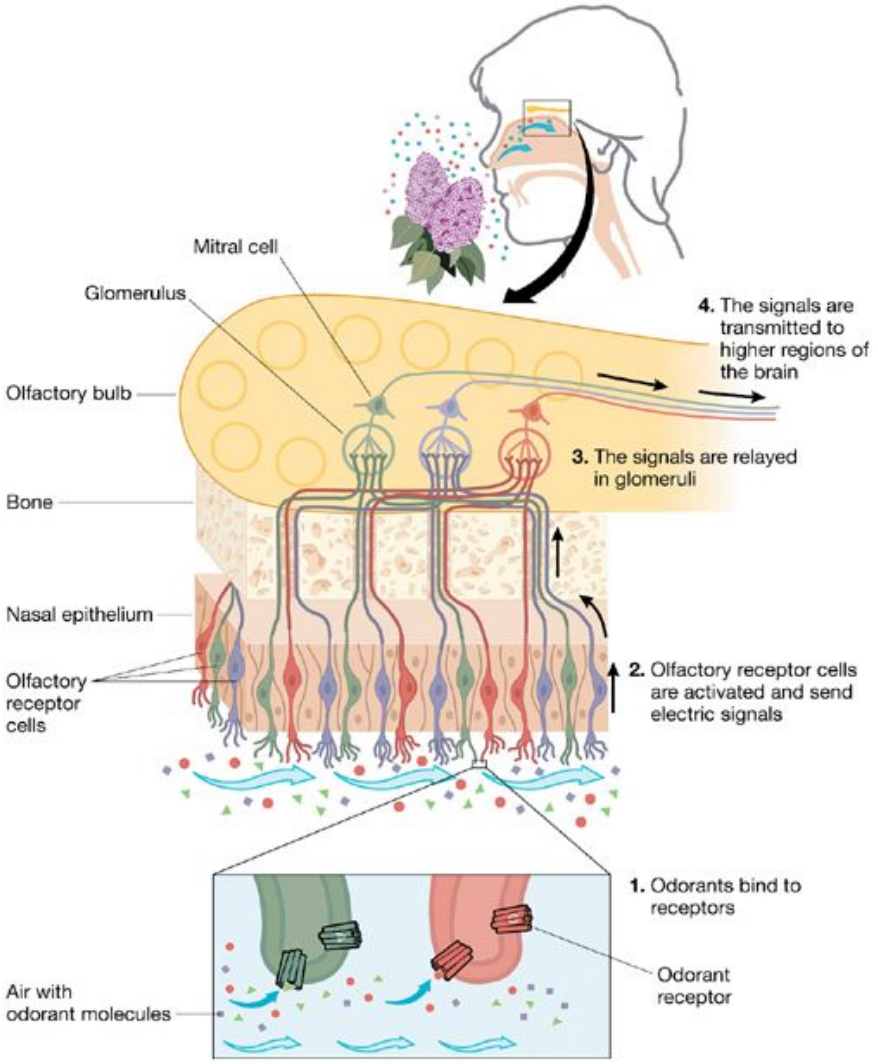
Orthonasal pathway

Aroma
(via mouth)

Retronasal pathway

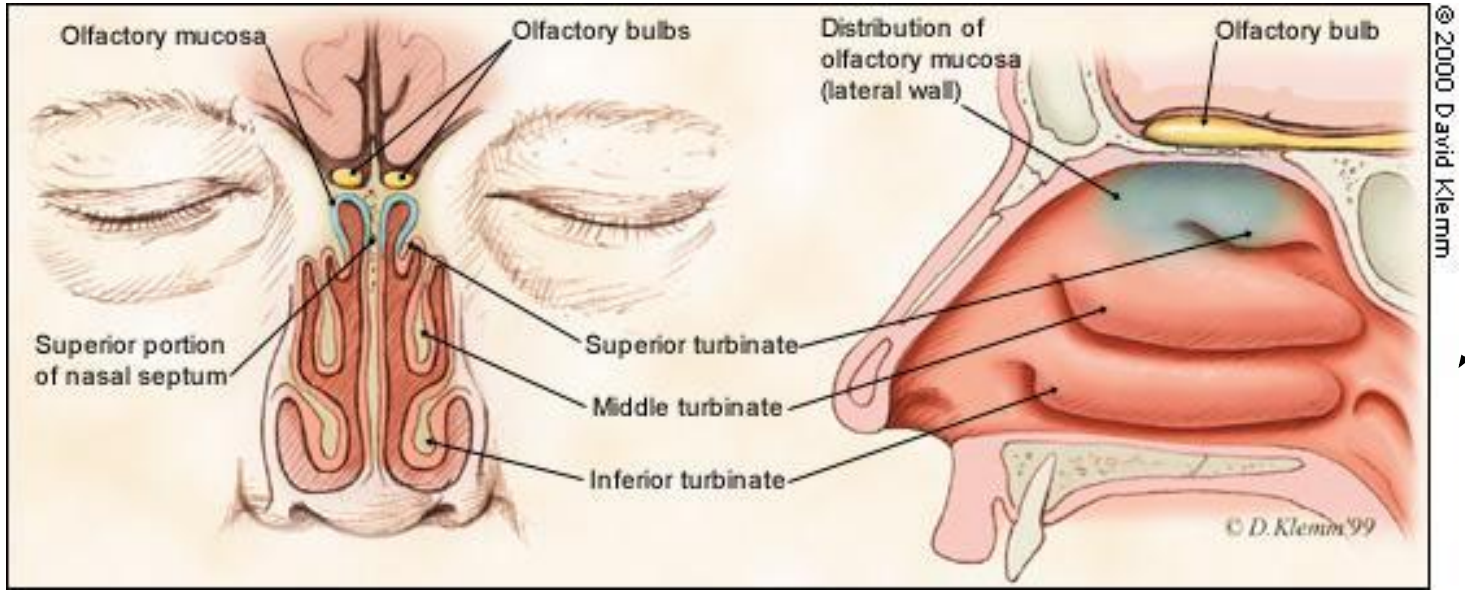
How does Olfaction work?

- Volatile aroma compounds detected by **olfactory receptor cells** – a type of specialised nerve cells (neurons).
- Cilia protruding into the nasal cavity increase surface area for binding.
- ORCs send a signal to the brain via the olfactory bulb.



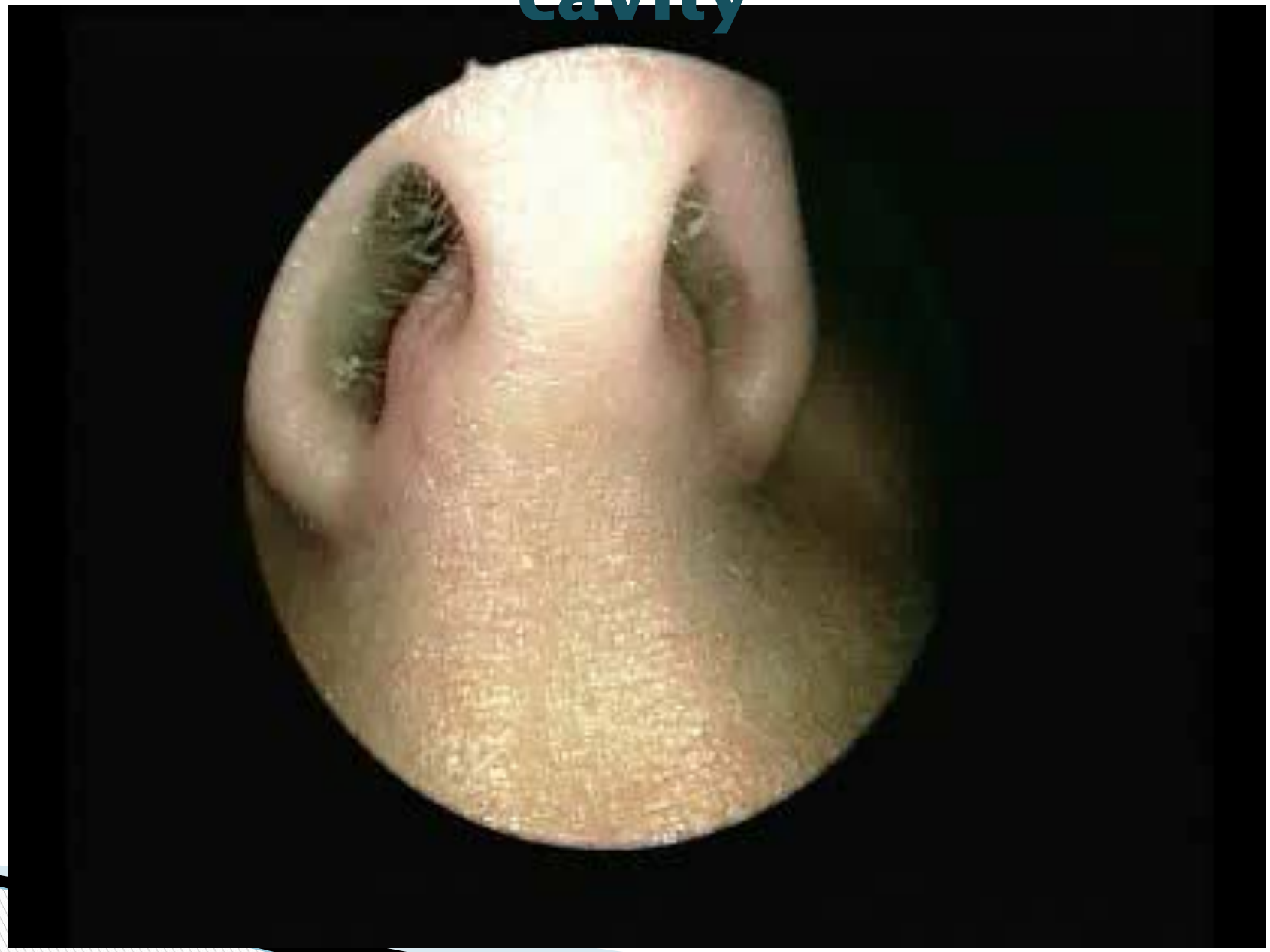
http://www.nature.com/embor/journal/v8/n7/fig_tab/7401029_F1.html (20/02/2012)

How does Olfaction work?



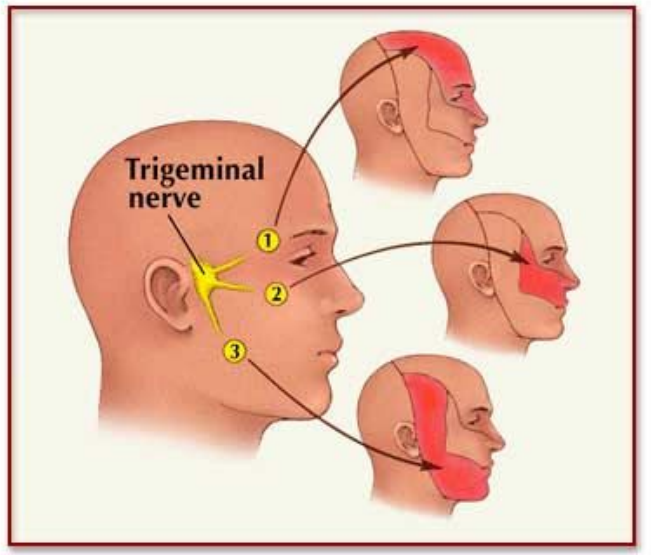
Nasopharynx

A journey through the nasal cavity

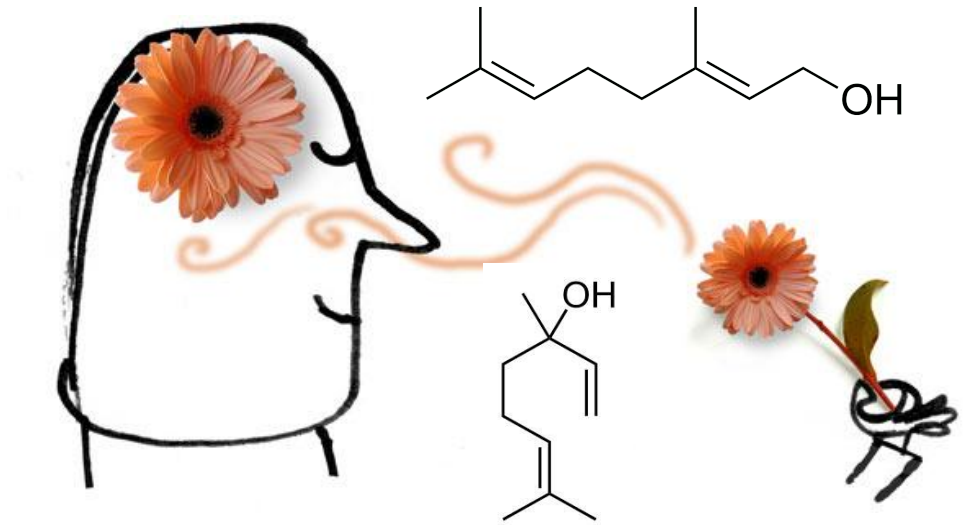


Chemesthesis (Chemical irritation)

- Chemically induced sensations detected in eyes, nose, mouth and external skin
  - Stimulate the trigeminal nerve
- Adds desirable characteristics and complexity to food
- Sensations
  - **Heat**: chilli
  - **Cooling**: menthol
  - **Pungency:** from wasabi, mustard, ginger, pepper
  - **Lachrymatory**: onions
  - **Irritation**: carbon dioxide



Flavour Chemistry



Odorants : Odour active compounds

- Defined as a compound that elicits an odour response
  - **Odour-active** or **flavour-active** aroma compounds
  - i.e. it impacts on FLAVOUR perception

- Thousands of volatile compounds have been identified in foods and natural products
  - E.g. >1000 in coffee, >500 hops, >200 strawberry

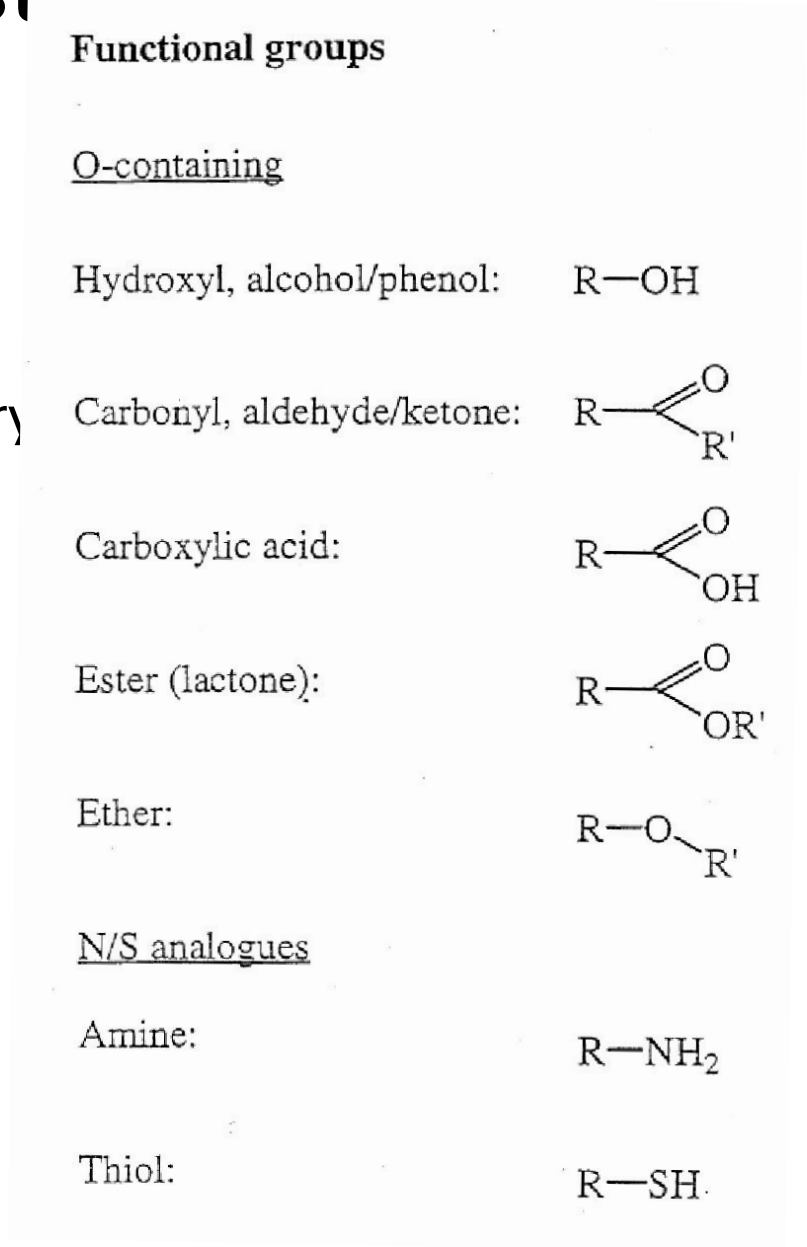
- Only a relatively small number of compounds are responsible for aroma perception
  - Demonstrates the specificity of olfactory receptors
  - Must be present in foods in concentrations above the odour threshold

Odorants

- **Character-impact odorants**
  - Key aroma compounds that are responsible for the **characteristic aroma** of the food / sample
    - Examples: Clove – eugenol; Thyme – thymol
  - The aroma of some samples is due to a complex mixture of aroma compounds
    - No single compound smells like the sample itself
    - e.g. coffee, hops, pineapple

Basic Flavour Chemistry

- **Classes of aroma compounds**:
  - Aroma compounds composed of carbon (C) and hydrogen (H) atoms backbones
  - **Odour activity** and **character** vary according to:
    - Chain length
    - Saturated vs unsaturated (i.e. double bonds)
    - Aliphatic (acylic) vs cyclic structures
    - Functional group
      - Usually oxygen containing
      - Sulfur and nitrogen analogues



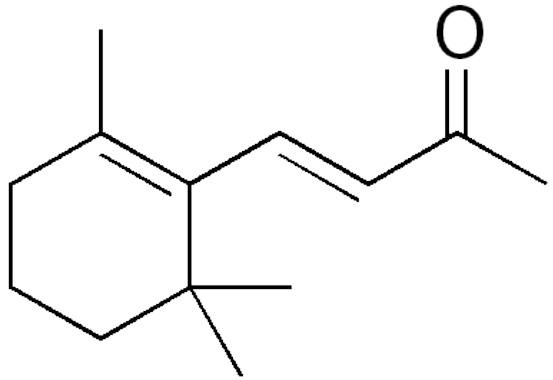
Odour thresholds

Aroma compound	Aroma character	Threshold in water at 20°C (mg/L)
Ethanol	Alcohol	100
Maltol	Caramel	9
Benzaldehyde	Almond, marzipan	0.35
Vanillin	Vanilla	0.02
Linalool	Floral, coriander	0.006
Hexanal	Cut grass	0.0045
Ethyl butanoate	Fruity	0.001
2-isobutyl-3-methoxypyrazine	Green, capsicum	0.000002
1-p-menthene-8-thiol	Grapefruit	0.00000002

Source: Belitz, Grosch & Schieberle, *Food Chemistry (4th Edition).* Springer, Berlin, 2009, p341.

β-Ionone

$(C_{13}H_{20}O)$



Odour: Floral, violet, fruity, berry

Origin: A degradation product from carotenoids

Occurrence: Flowers, fruits, vegetables, wine

Anosmia: The total loss of the sense of smell (olfaction).

Specific Anosmia: The inability to smell a specific chemical compound.

About **37%** of the population cannot smell **β-ionone**.

Can you smell it??

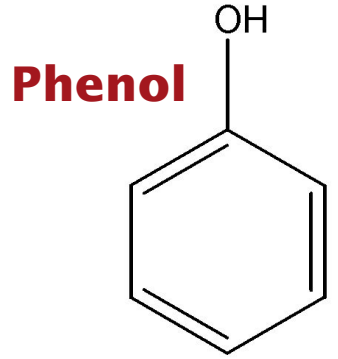
Aroma Compounds

- **Alcohols**
  - Derived from fatty acids and amino acids
    - By products of metabolism reactions
  - Also produced in fermentation as a by product of **amino acid metabolism**
  - Contributes **alcoholic**, **spicy**, **wine-like** (vinous) and attributes.
  - Examples:
    - Amyl alcohol (alcoholic, marzipan) – Isoleucine
    - Isoamyl alcohol (alcoholic, whiskey) – Leucine
    - Isobutanol (alcoholic, fruity) – Valine
    - 2-phenylethanol (floral, rose) – Phenylalanine

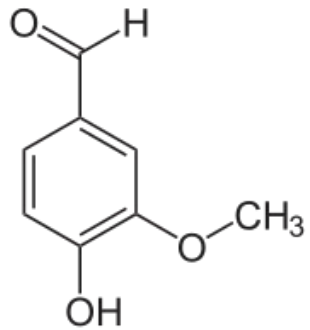
C-OH

Aroma Compounds

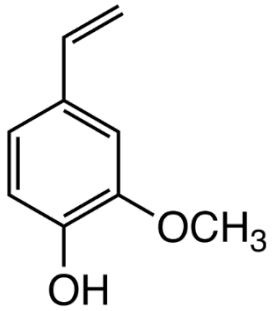
- **Phenols**
  - Found in plants, smoked/roasted products, and fermented products
  - Plant derived:
    - Eugenol – clove oil
    - Vanillin – in vanilla
  - Smoked / roasted products
    - E.g. Guaiacol (2-methoxyphenol)
  - Produced by **specialty yeast strains**
    - German wheat beers; Belgian specialty beers
    - Contribute spicy, peppery, clove, medicinal characters.
      - E.g. 4-vinyl guaiacol
  - Also responsible for various off-flavours



Phenol



Vanillin



4-vinyl guaiacol

Aroma Compounds

- **Aldehydes**
  - Commonly found in fruits, leaves and vegetables
  - Derived from both fatty acids and amino acids
    - By products of metabolism reactions
    - Products of lipid oxidation (rancidity)
    - Generated by heat during cooking (Strecker aldehydes from Maillard reaction)
  - Responsible for **green**, **'fresh'**, **unripe**, **waxy**, **citrus** characters
  - Examples:
    - Hexanal, *E*-2-hexenal (**cut grass**) – tomatoes, apple
    - Decanal (**citrus peel**)
    - *(E,Z)*-(2,6)-Nonadienal (**cucumber**)
  - Impact odorants in coriander leaf – unsaturated aldehydes
  - Also found in melons, pumpkin, etc.
  - Also key odorants in Chanel No. 5 perfume

CH=O

Individual Perception and Preference

- Unsaturated aldehydes are also the impact odorants in **coriander leaf (Cilantro)**
  - e.g. *E*-2-decenal
- Well documented prevalence of consumers who strongly dislike coriander leaf due to ***genetics***

Fresh, fragrant, citrusy

Stinkbug!
Soapy, chemical
3-21% of consumers

Aroma Compounds

- **Ketones**
  - Commonly found in cheese and dairy products
  - Produced by microorganisms
  - Examples:
    - 2-heptanone (**blue cheese**)
    - Diacetyl (**buttery**)

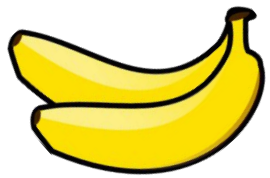
C=O

- **Carboxylic acids**
  - Commonly found in cheese and dairy products
  - Lipid hydrolysis and oxidation
  - Examples:
    - Butanoic (butyric) acid (baby vomit, rancid, parmesan cheese)
    - Isovaleric acid (sweaty, cheesy)

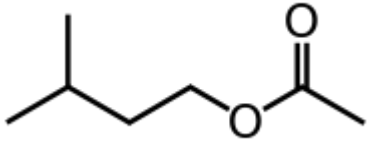
COOH

Aroma Compounds

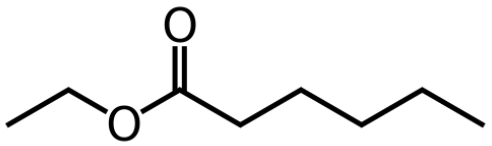
- **Esters**
  - Widespread in nature, fruits, fermented beverages etc.
    - Alcohol and carboxylic acid linked by ester bond
  - Responsible for **fruity** characters
  - Very important as commercial flavour compounds
  - Examples:
    - Isoamyl acetate (banana)
    - Ethyl butanoate (berry)
    - Ethyl hexanoate (pineapple)



Isoamyl acetate



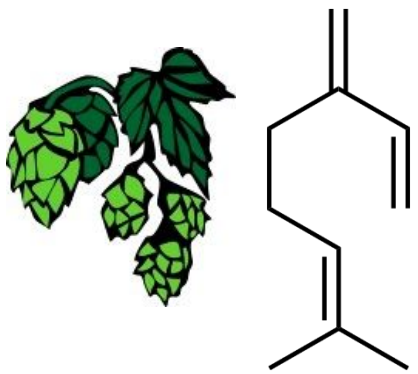
Ethyl hexanoate

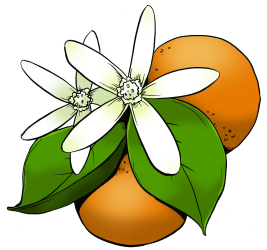


Aroma Compounds

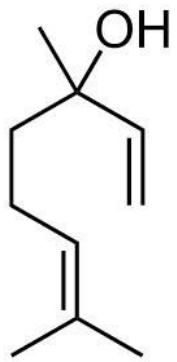
- **Terpenes**
  - Large, complex class of organic compounds produced by plants.
  - Examples:
    - Monoterpene hydrocarbons, e.g. pinene, myrcene
    - Monoterpene alcohols, e.g. linalool (floral, citrusy)
    - Monoterpene aldehydes, e.g. citral (lemony)

Myrcene
Green, resinous

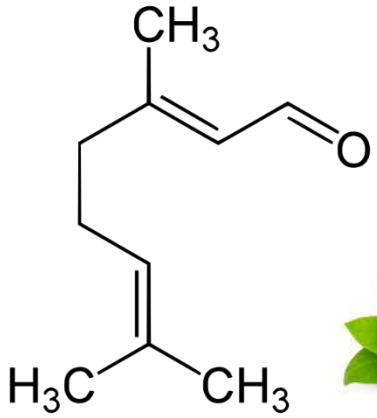




Linalool
Floral, citrusy



Citral A
Lemon zest

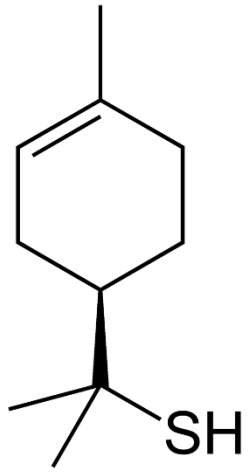


Polyfunctional thiols

- Higher MW sulfur compounds with oxygenated functional groups.
- Found to be important impact odorants in fruits (passionfruit, grapefruit), wine, hops and beer etc.

Grapefruit mercaptan

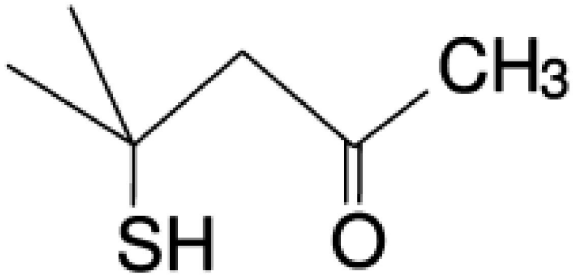
(1-*p*-menthene-8-thiol)



Odour character:
Grapefruit

4MMP

(4-methyl-4-mercapto-2-pentanone)



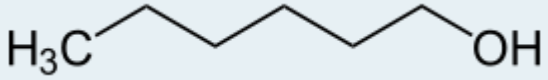
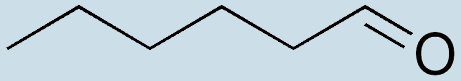
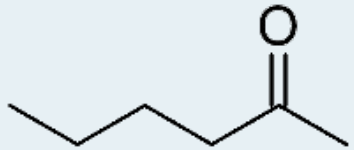
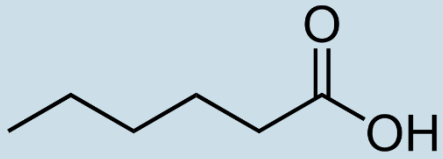
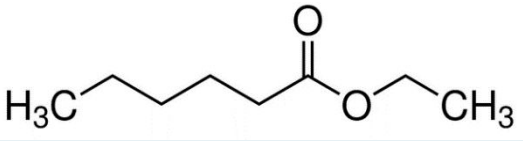
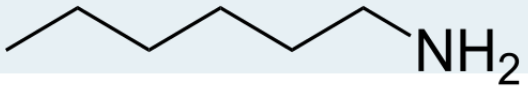
Odour character:
Cat pee, blackcurrant, box tree

Others… many!!

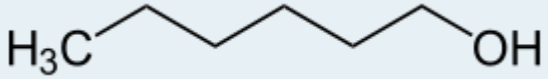
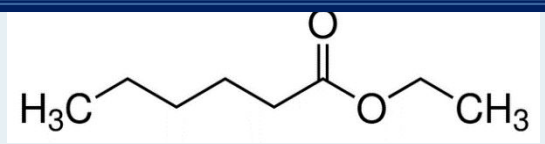
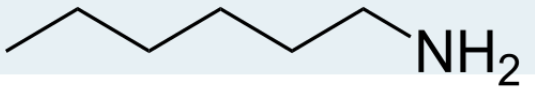
- E.g. Products of caramelisation and the Maillard reaction
- Caramel aroma compounds
  - Complex set of reactions and chemical products
    - E.g. Pyrazines, Pyrroles, Furanones
  - Generates flavour attributes such as caramel, toffee, toasted, roasted, nutty etc.



Structure – Odour relationships

Class	Compound	Structure	Odour
Alkane	Hexane		Solvent
Alcohol	Hexanol		Alcohol
Aldehyde	Hexanal		Green, grass
Ketone	2-Hexanone		Blue cheese
Carboxylic acid	Hexanoic acid		Cheesy, sweaty
Ester	Ethyl hexanoate		Fruity, pineapple
S-containing	Hexanethiol		Metallic, meaty
N-containing	Hexyl amine		Fishy, musty

Structure – Odour relationships

Class	Compound	Structure	Odour
Alkane	Hexane		Solvent
Alcohol	Hexanol		Alcohol
Aldehyde			Green, grass
Ketone			Blue cheese
Carboxylic acid			Cheesy, sweaty
Ester	Ethyl hexanoate		Fruity, pineapple
S-containing	Hexanethiol		Metallic, meaty
N-containing	Hexyl amine		Fishy, musty

Chemistry dictates odour character and physico-chemical properties

Summary

- **Flavour** is a complex, integrated perception interpreted in our brain.
  - Composed of individual sensations odour, aroma, taste, texture/mouthfeel and chemesthesis.
- **Flavourings** are ingredients added to foods to enhance sensory properties.
  - Primarily **aroma compounds**.
- Wide variety of aroma compounds found in nature and in foods.
  - **Odour activity** and **character** vary according to chemical structure
  - Small changes in the structure or functional groups can have a major impact

Flavour Research at Otago

Research Question

How can we use **volatile analysis and sensory science** to understand **flavour perception**?

University of Otago
ŌTĀKOU WHAKAIHU WAKA

Integrated Capability: Through Chain Approach

Raw materials

Advanced Processing
Emerging Technologies

Drivers of liking

Milk / Dairy

Fruits / Vegetables

Grains / cereals

Meat / Seafood

Sensory Perception

Composition

Food Waste
By-product utilisation

Health

Food Choice and Eating behaviour

Raw Materials

Processing

Flavour Chemistry	Sensory	Consumer
• Composition analysis • Flavour generat • Volatile Analysis • Flavour Release	• Characterise sensory	• Drivers of consumer umer ption of quality • Food choice behaviour

Target Outcome
Optimise food quality

Product Innovation

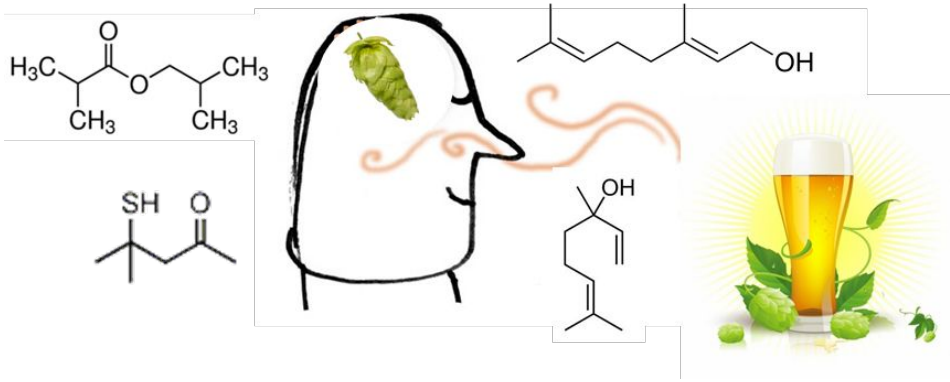
Health

What is responsible for the aroma of hops?

UNIVERSITY of OTAGO
Te Whare Wānanga o Otāgo
NEW ZEALAND

Research Question

What are the compounds responsible for aroma characters in New Zealand hop varieties?

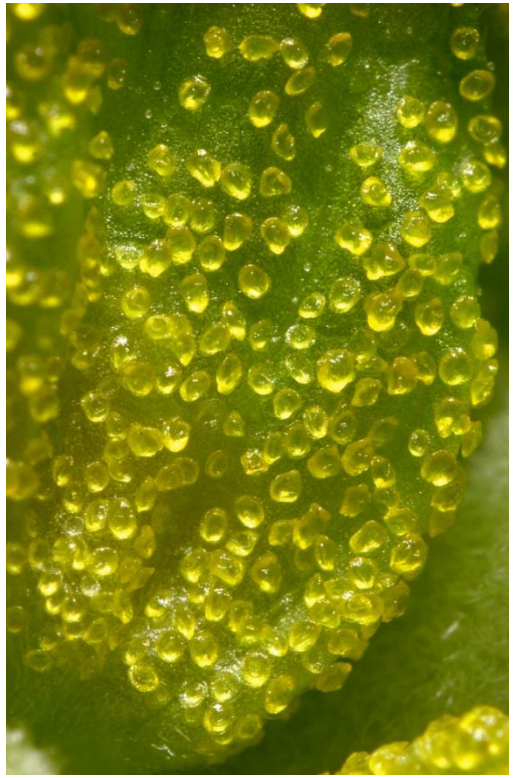


Support Hop Breeding in New Zealand

Hops (*Humulus lupulus*)

Purpose of adding hops:

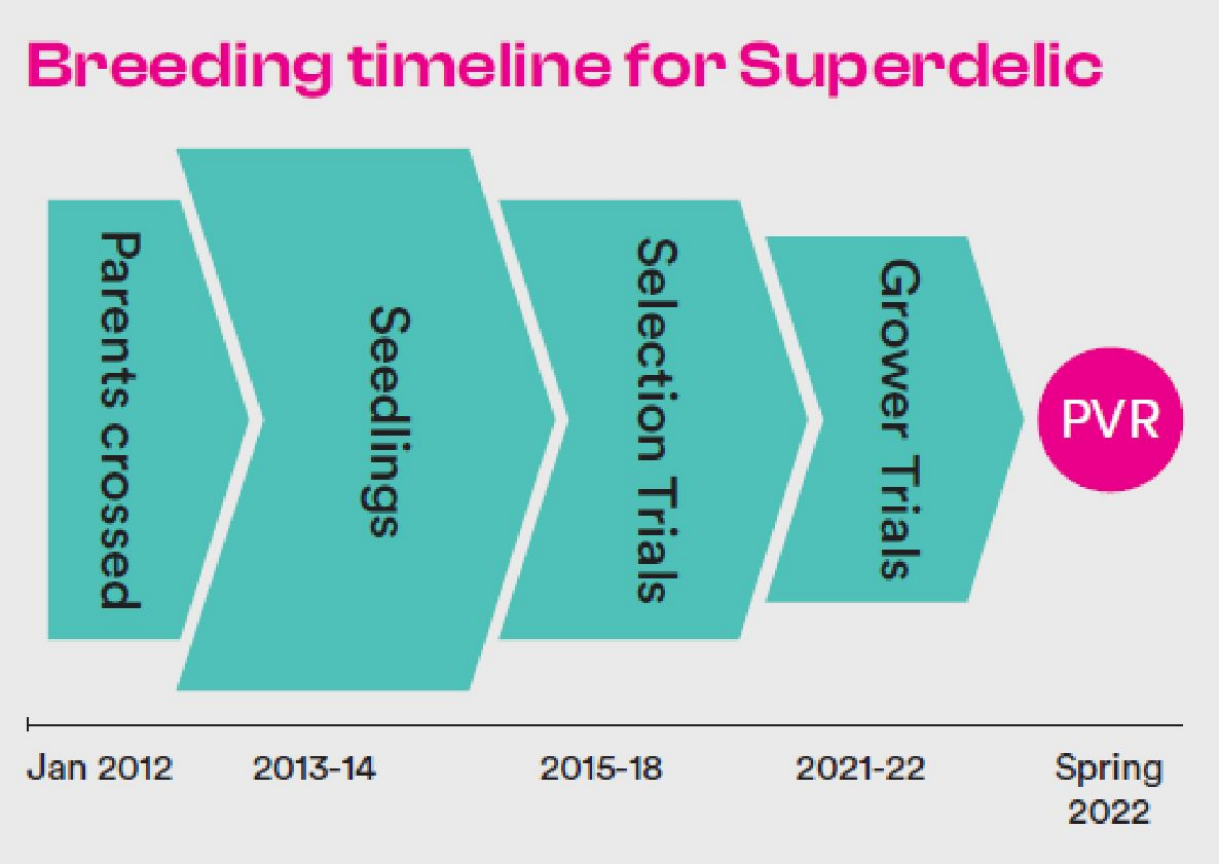
- Provide **bitterness**
  - Essential to balance malt sweetness and give beer its refreshing drinkability
- Provide **flavour and aroma**
- Provide an **antimicrobial effect** to help preserve the beer.

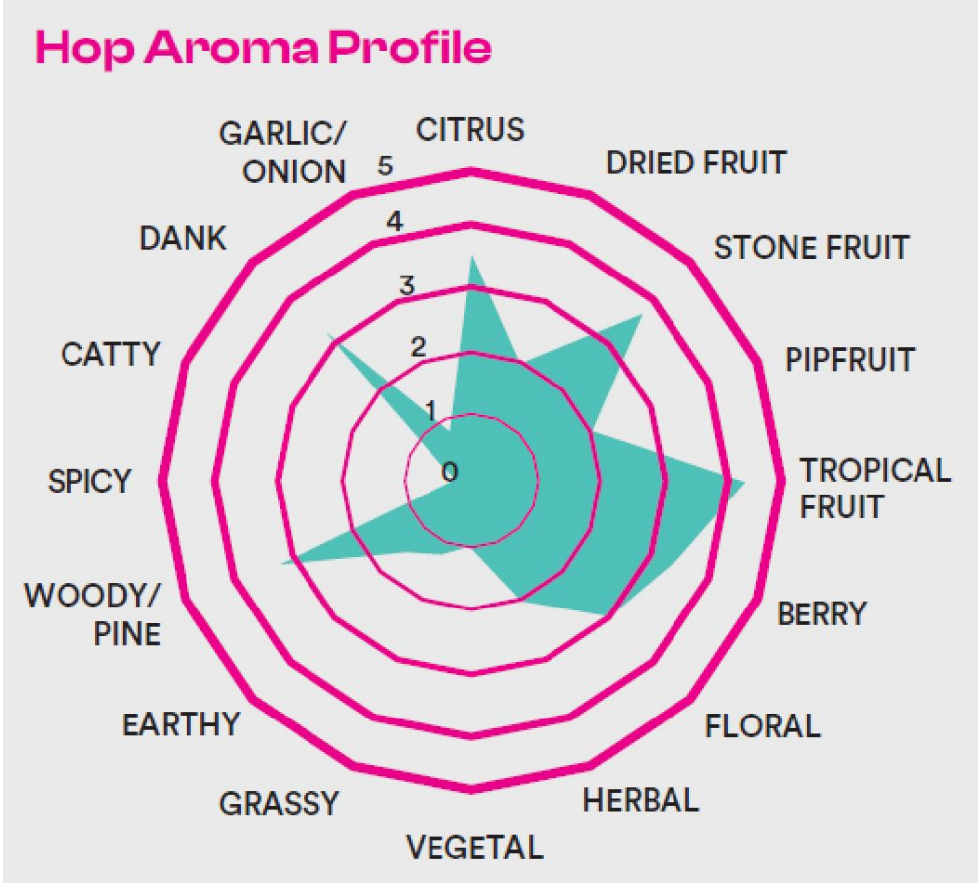


New Cultivar: Superdelic (2023)

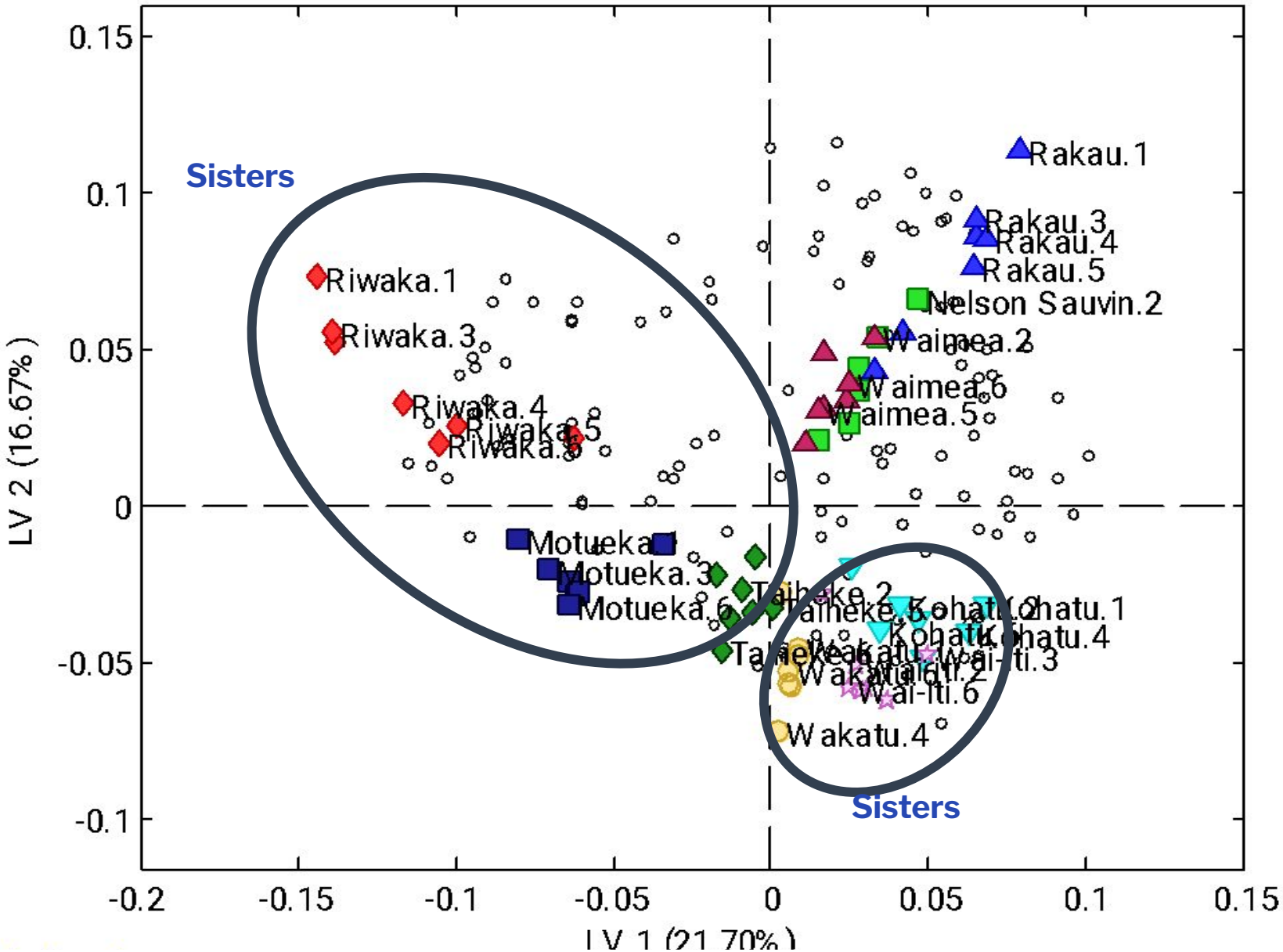
https://nzhops.co.nz/blogs/news/new-hop-release-nz-hops-ltd-unveils-superdelic%E2%84%A2

New Cultivar: Superdelic (2023)



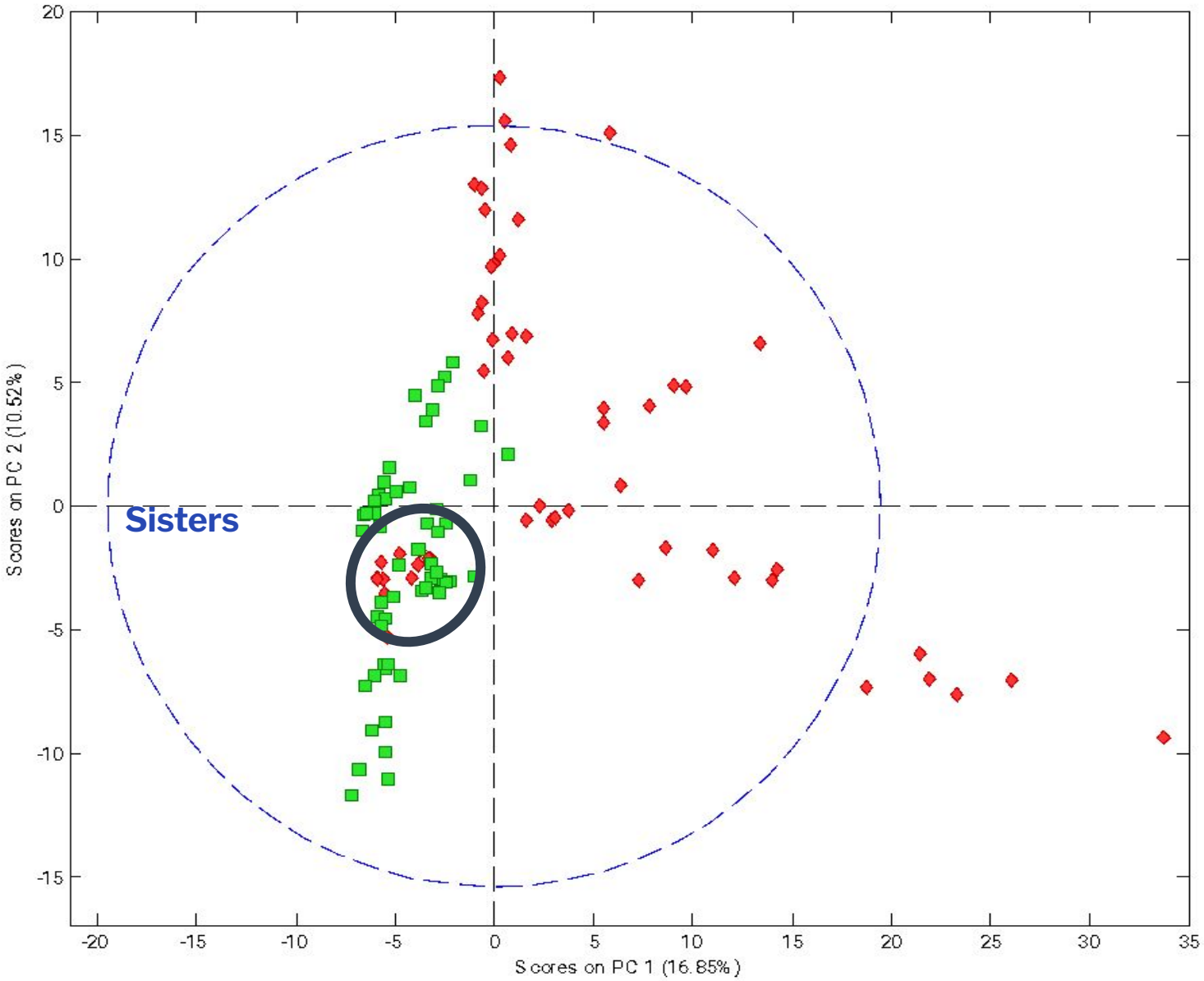


Commercial Hop Cultivars



- Volatile analysis is used to identify discriminating cultivars
- Identify marker compounds
- Monitor quality and authenticity

Advanced Selections



- Volatile analysis is used to screen new breeding selections for their chemical profile (phenotype)
- Used to distinguish and select new cultivars
  - Marker compounds

Hop Growing Locations

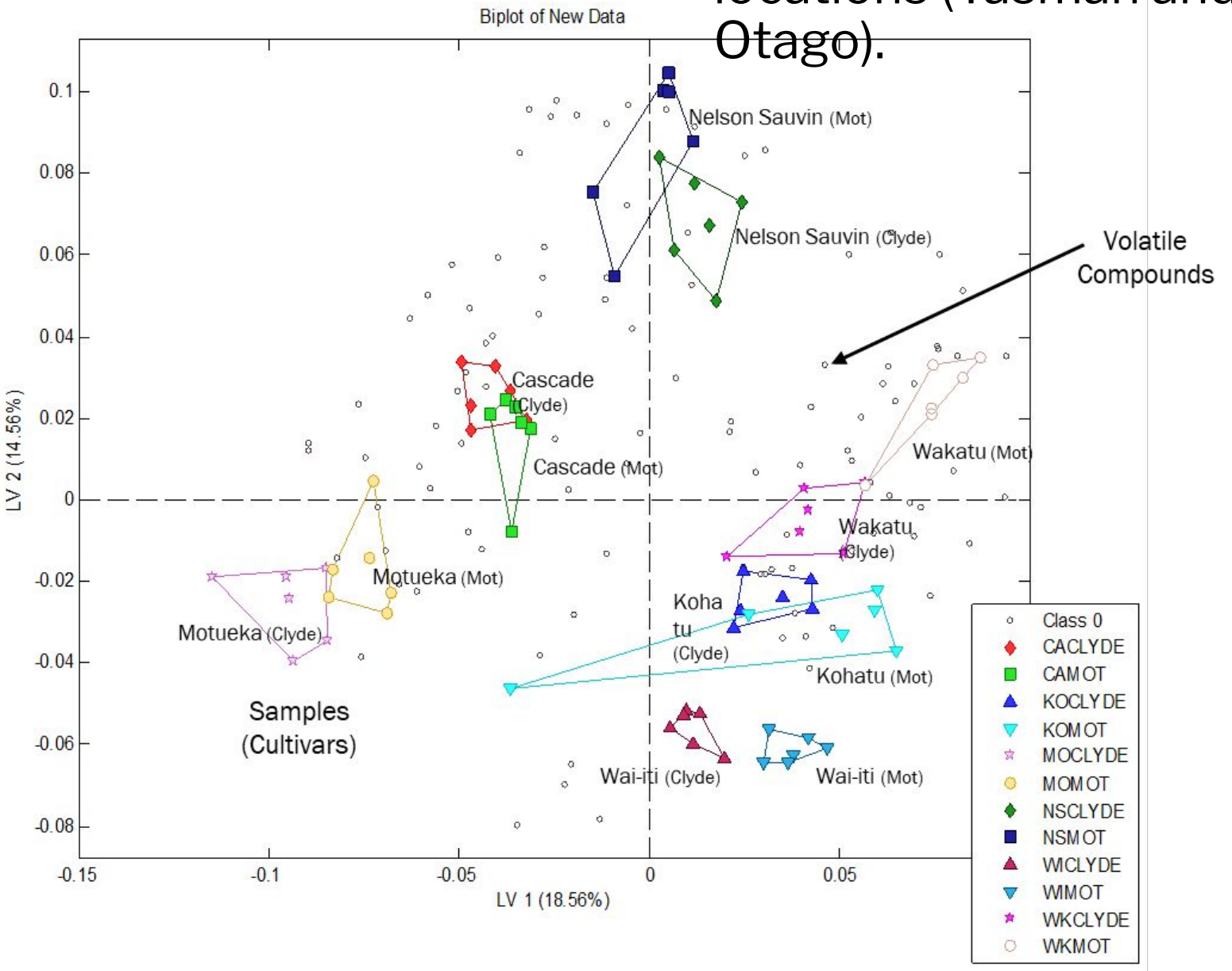
- Optimal growth conditions are required to produce economically viable hops
- **Growth conditions**:
  - Long daylight hours
  - Warm summer sun
  - Periods of winter cold
  - Deep & fertile soil
  - Regular water
  - Shelter from the wind
- Hops are a **latitude sensitive** crop
  - Cultivation between 35° and 55°

Growing Regions

- Commercial production focussed in the Tasman region.
- Competition for land and resources
  - Grapes for wine
  - Kiwifruit
  - Pipfruit
- Need for new growing locations to expand the industry and meet increasing demand.
- ***What about Central Otago?***

Hop Terroir?

Differences in chemical profile of hop cultivars from two growing locations (Tasman and Central Otago).



- Hop cultivar (**genetics**) has the greatest impact on chemical profile.
- **Hops can be successfully grown in Central Otago and recognised as the same variety.**
- Subtle differences.
- Demonstrates the potential to expand

Summary

- Hops are a small but growing horticultural industry in New Zealand
- Rich history of successful breeding
- Current breeding scheme is applying research and innovation according to **phenotype targets**
  - Disease resistance
  - Agronomy factors
  - Sensory profile – Aroma and flavour
  - Chemical Profile – molecular target compounds

Acknowledgements

Thank you for your attention!

Thanks to:

Ron Beatson (Plant and Food Research Ltd; NZ Hops)

Victoria Purdy (PhD Student)

Esther Fogarty (Hons Student)

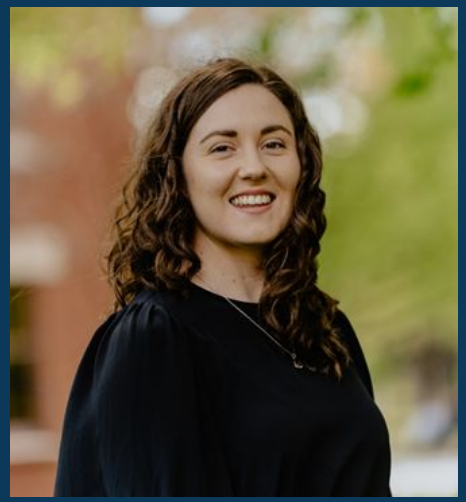
Pat Silcock and Biniam Kebede

A/Prof Graham Eyres

Department of Food Science

University of Otago

graham.eyres@otago.ac.nz



Thank you for your Attention

Contact:
A/Prof Graham Eyres
Department of Food Science
University of Otago
graham.eyres@otago.ac.nz

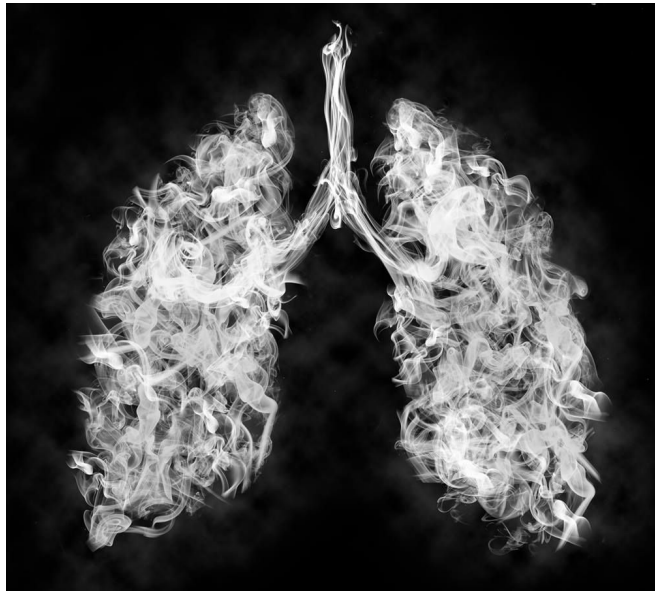
Te Tari Pūtaiao Kai
Ōtākou Whakaihu Waka

Example: Coriander *(Coriandrum sativum)*

- Immature leaves – ***Herb***
- Dried fruit (coriander 'seed') – ***Spice***
- Roots?

Flavours in Vaping liquids

- Vaping involves heating an e-liquid into an **aerosol** or vapour cloud that is inhaled by the user.
- E-Liquids contain:
  - Nicotine
  - Propylene glycol
  - Vegetable glycerine (glycerol)
  - Flavours
- Promoted as a smoking cessation tool to lower **Risk**
- Is it 'Safe'?
  - "Less Harmful" or "lower risk" does not mean "***Safe***"



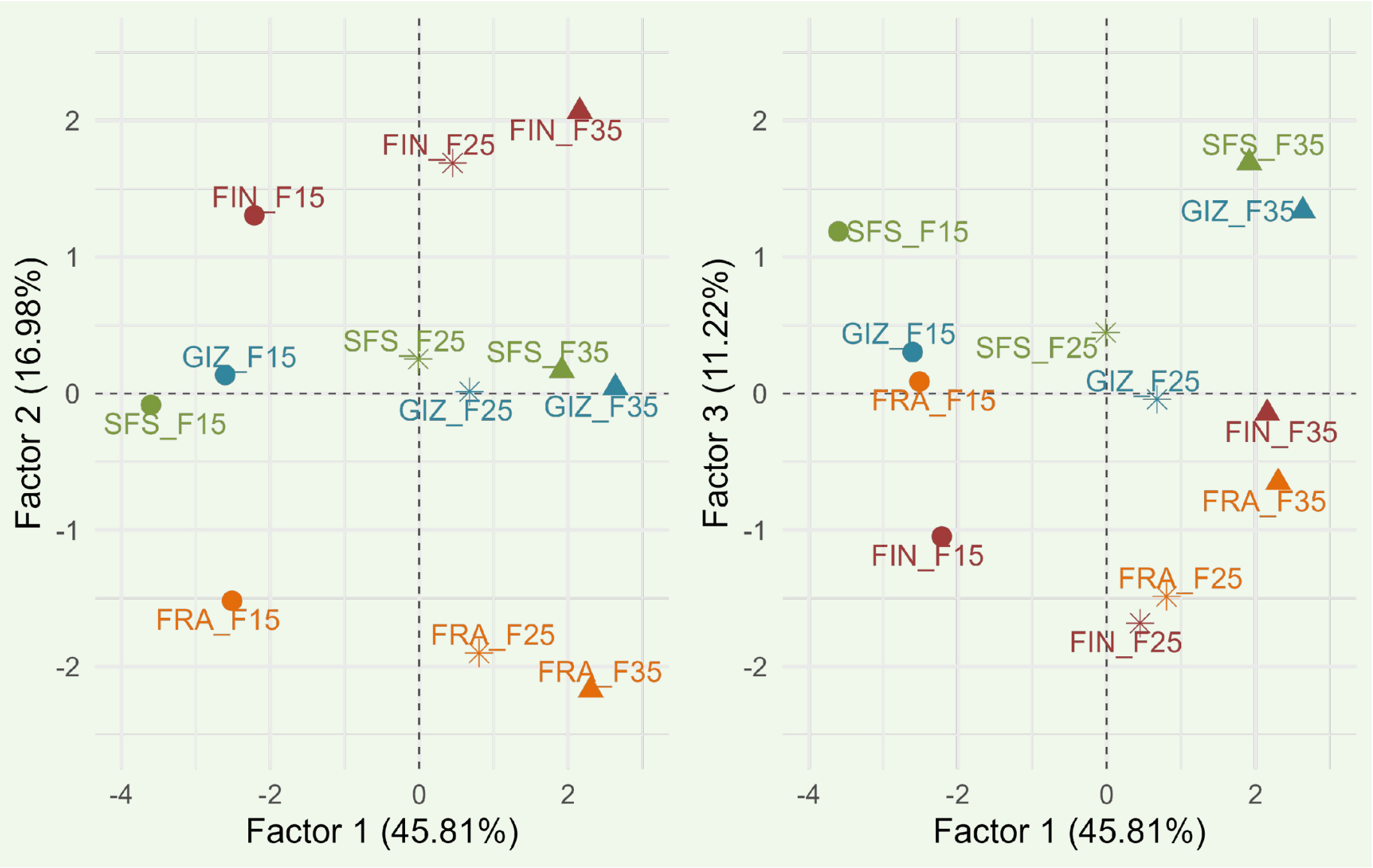
Safety of Flavours in Vaping

- Current regulations for flavours are based on the **Food Standards Code**
  - Same list of permitted compounds with GRAS status
  - But… this is based on **Ingestion** not **Inhalation**

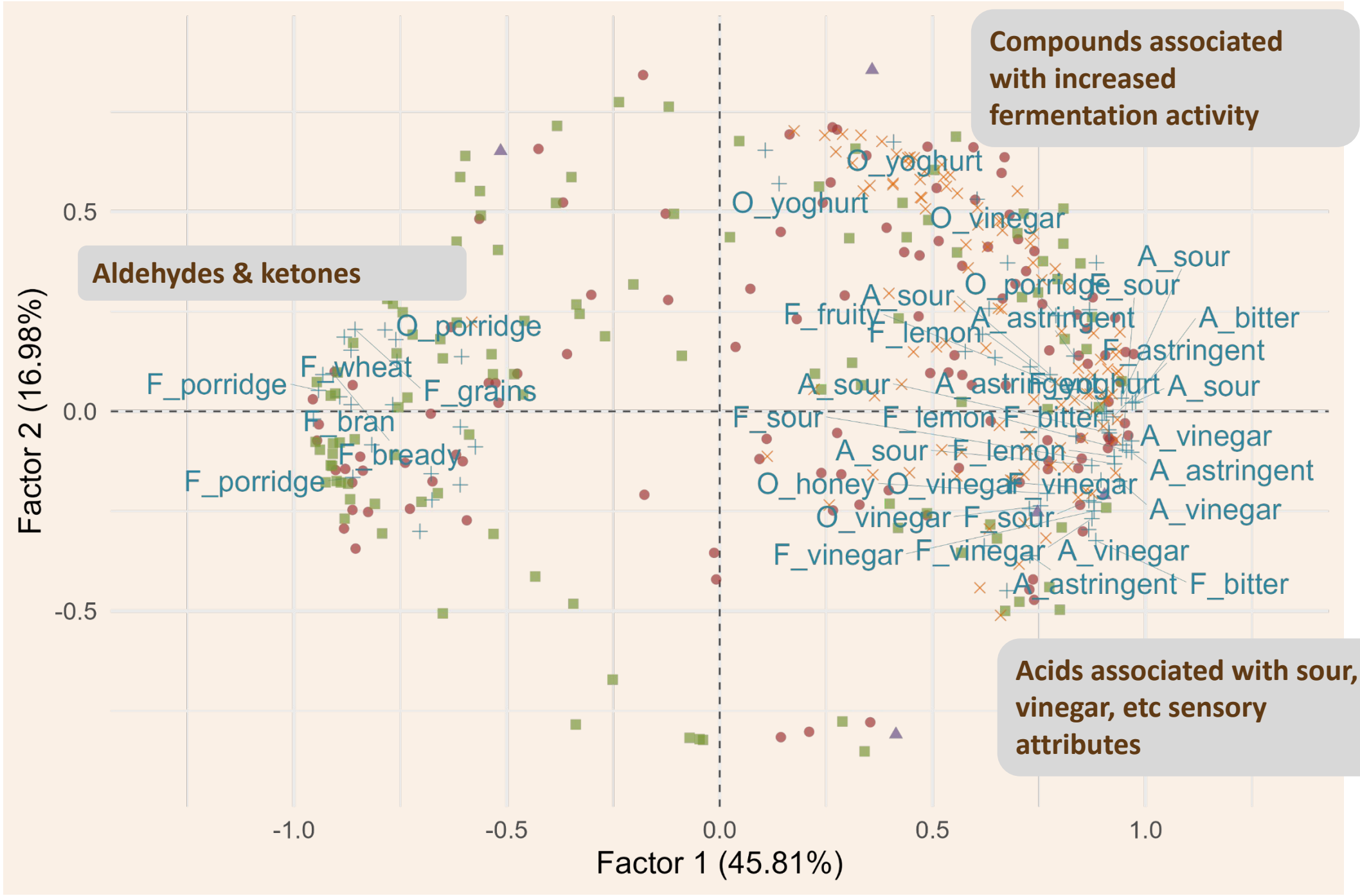
- There is no specific information on the composition of products in NZ.

- The long-term safety and health impacts of the flavour compounds associated with **inhalation** during vaping **is not known**.

MFA all data

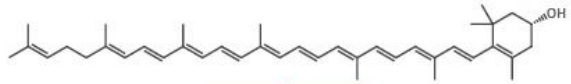

FIN_F25
FIN_F35
FIN_F15
SFS_F25
SFS_F35
GIZ_F15
GIZ_F25
GIZ_F35
SFS_F15
FRA_F15
FRA_F25
FRA_F35
Factor 2 (16.98%)
Factor 1 (45.81%)
SFS_F35
GIZ_F35
SFS_F15
GIZ_F15
SFS_F25
GIZ_F25
FRA_F15
FIN_F35
FRA_F35
FIN_F15
FRA_F25
FIN_F25
Factor 3 (11.22%)
Factor 1 (45.81%)

MFA Attribute Loadings

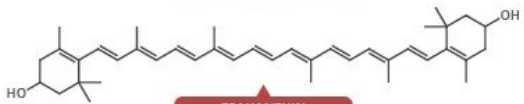


THE COLOUR AND AROMA OF ROSES

THE COLOURS OF ROSES



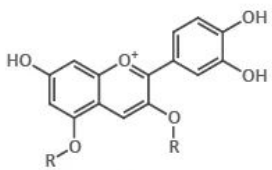
RUBIXANTHIN



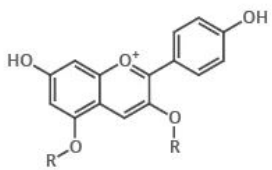
ZEAXANTHIN

Other carotenoids include lutein, lycopene, beta-carotene, taraxaxanthin, and rosaxanthin

Roses come in a variety of colours, and different chemical pigments are responsible for the different shades. A large variety of carotenoids (above) give yellow and orange hues, while a smaller number of anthocyanins (below) give the more typical reds. Combinations of compounds from the two classes of pigments give the variety of different shades of these colours.



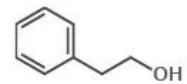
CYANIN



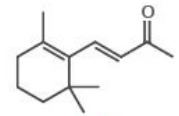
PELARGONIN

R groups = glucose (in both molecules)

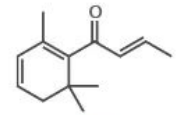
THE AROMA OF ROSES



2-PHENYLETHANOL

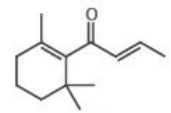


β-IONONE

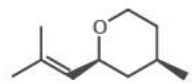


β-DAMASCENONE

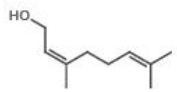
The aroma of roses is contributed to by a number of different chemical compounds; some key contributors are shown here. Their contribution to the aroma varies and isn't tied to their concentrations; in fact a number of them have very low concentrations! Important contributors are rose ketones (including damascenones, damascones, and ionones) and (-)-*cis*-rose oxide.



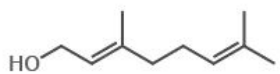
β-DAMASCONE



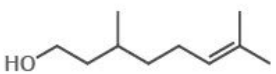
(-)-*cis*-ROSE OXIDE



NEROL



GERANIOL



CITRONELLOL