Examples of food chemistry molecules

Borrowed from Compound Interest, the amazing work of Andy Brunning, UK science educator
https://www.compoundchem.com/category/food-chemistry/

COFFEE CHEMISTRY: ARABICA VS ROBUSTA

ARABICA COFFEE BEANS

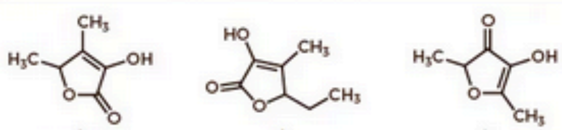
WORLD PRODUCTION

- ALTITUDE 600–2200m
- RAIN 1200–2200mm
- TEMPERATURE 15–24°C

CAFFEINE CONTENT
1.2–1.5%

CHLOROGENIC ACID CONTENT	5.5–8.0%
LIPID (FAT) CONTENT	15–17%
SUGAR (SUCROSE) CONTENT	6.0–9.0%

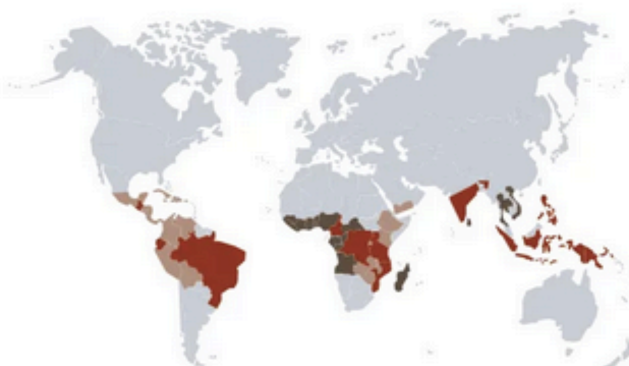
KEY FLAVOUR COMPOUNDS



SOTOLON · ABHEXON · FURANEOL

These compounds give the coffee sweet caramel notes

Arabica produces less coffee per hectare than robusta, and is consequently more expensive. It is also more susceptible to disease.



- Regions in which arabica is primarily grown
- Regions in which robusta is primarily grown
- Regions in which arabica and robusta are grown

ROBUSTA COFFEE BEANS

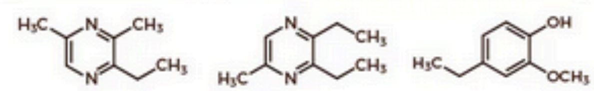
WORLD PRODUCTION

- ALTITUDE 0–800m
- RAIN 2200–3000mm
- TEMPERATURE 18–36°C

CAFFEINE CONTENT
2.2–2.7%

CHLOROGENIC ACID CONTENT	7.0–10.0%
LIPID (FAT) CONTENT	10.5–11.0%
SUGAR (SUCROSE) CONTENT	3.0–7.0%

KEY FLAVOUR COMPOUNDS



3,5-DIMETHYL-2-ETHYLPYRAZINE · 2,3-DIETHYL-5-METHYLPYRAZINE · 4-ETHYLGUAIACOL

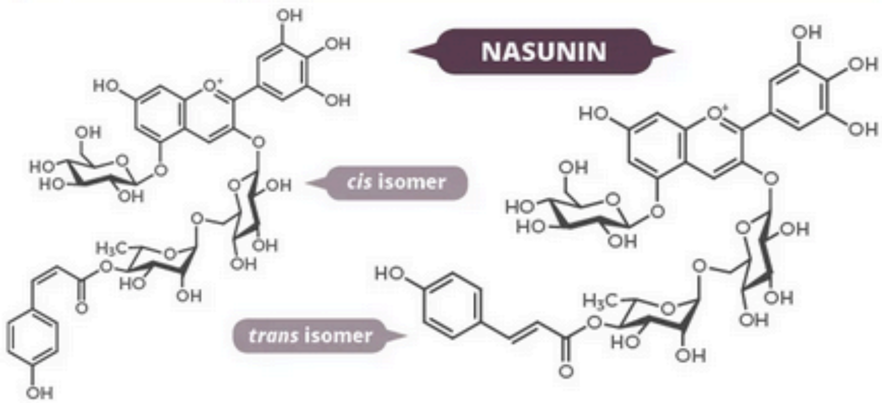
These compounds give the coffee spicy, earthy notes

Robusta is considered to have a harsher, more bitter flavour compared to the smoother flavour of arabica. It is often used in blends.

THE CHEMISTRY OF EGGPLANTS

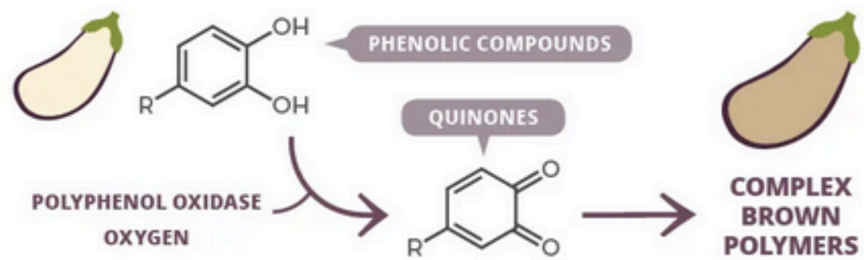
THE COLOUR AND TEXTURE OF EGGPLANTS

The purple colour of eggplants comes from anthocyanin pigments. The main anthocyanin present is nasunin, named after the Japanese name for eggplant ('nasubi'). It is present as a mix of *cis* and *trans* isomers; the *trans* isomer is the more stable of the two.



Eggplants have a spongy texture, caused by many tiny air pockets between cells. This is why they shrink when cooked, and also soak up cooking oil. The latter can be prevented by pre-cooking or adding salt to draw out water into the air pockets, collapsing the structure.

BITTER FLAVOUR AND BROWNING



Phenolic compounds cause the bitter flavour of eggplants. These compounds also explain their browning when cut. Cutting releases polyphenol oxidase enzyme from cells; it oxidises phenolic compounds, leading to the eventual formation of brown polymers.

THE CHEMISTRY OF SPINACH

THE IRON CONTENT OF SPINACH

Compared to many other vegetables, spinach does have a higher iron content. However, iron in vegetables tends to have low bioavailability – that is, it is not easily absorbed in the body.

SPINACH

2.6mg per 100g

1.7% ABSORBED

0.044mg

SIRLOIN STEAK

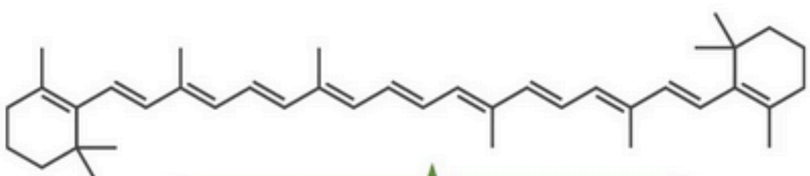
2.5mg per 100g

20% ABSORBED

0.50mg

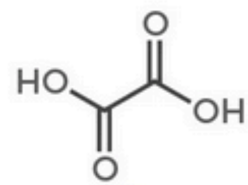
Sources: USDA food composition database; Scrimshaw (1991)

Low absorption of iron is partly due to polyphenol compounds in spinach binding iron – not due to its oxalic acid content (as previously thought). Though it might not be a great source of iron, it's a good source of vitamin A in the form of carotenoids.

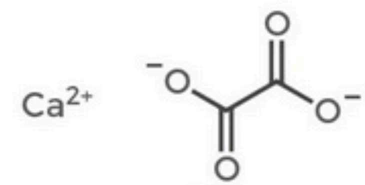


β-CAROTENE – VITAMIN A PRECURSOR

WHAT CAUSES 'SPINACH TEETH'?



OXALIC ACID



CALCIUM OXALATE

Spinach contains high amounts of oxalic acid. When you eat spinach, it can leave your teeth with a 'chalky' feel. This is caused by the oxalic acid reacting with the calcium ions in the spinach and in your saliva. This forms poorly soluble calcium oxalate crystals which coat your teeth.

THE CHEMISTRY OF COW'S MILK

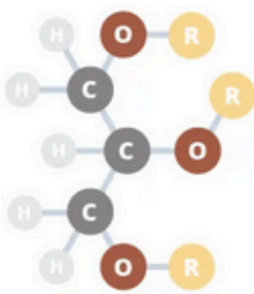
MILK'S COMPOSITION

Milk is an emulsion of fat in water. It is also a colloidal suspension of proteins. Other compounds, including lactose and minerals, are fully dissolved in the solution.

WATER	87.5%
FAT	3.9%
PROTEINS	3.4%
LACTOSE & MINERALS	5.2%

FATS IN MILK

Droplets of fat in milk have an average size of 3–4 micrometres. They consist mainly of triglycerides, and also contain fat-soluble vitamins.



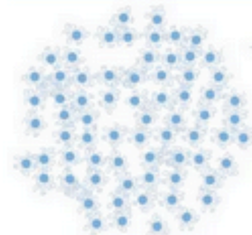
TRIGLYCERIDE

R = FATTY ACID MOLECULES

PALMITIC ACID	23.6–31.4%
OLEIC ACID	14.9–22.0%
STEARIC ACID	10.4–14.6%
MYRISTIC ACID	9.1–11.9%

WHY IS MILK WHITE?

Milk contains hundreds of types of protein, of which casein is the main type. The milk proteins form micelles. These micelles scatter light, causing milk to appear white.



CASEIN MICELLES

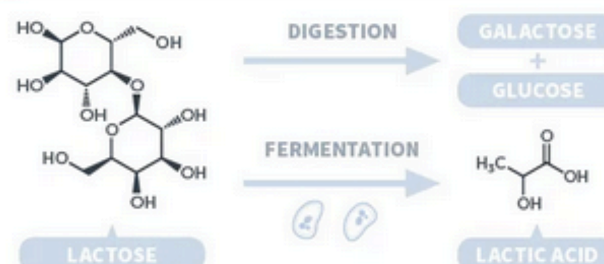
There are several models of casein micelle structure. This diagram shows the supramolecular structure.

CASEIN PROTEINS

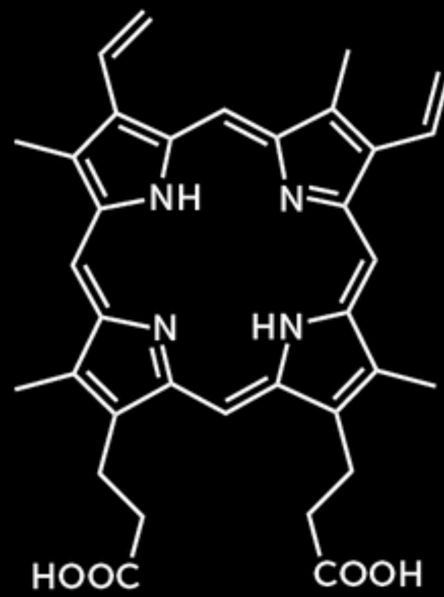
CALCIUM PHOSPHATE CLUSTER

LACTOSE & MILK

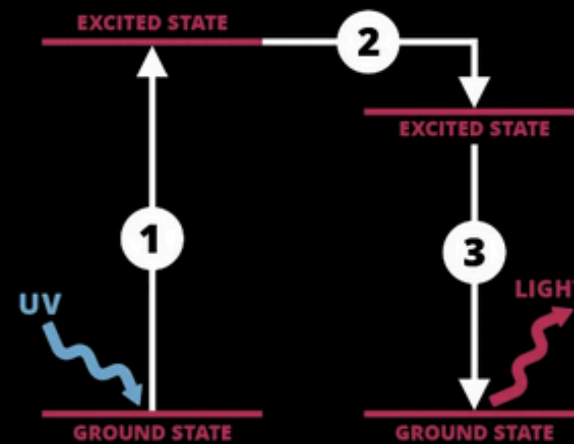
Lactose is a sugar found in milk. People who are lactose intolerant are unable to digest it. Lactose can be fermented by microorganisms to form lactic acid, causing the milk to sour.



THE CHEMISTRY OF EGG FLUORESCENCE



PROTOPORPHYRIN IX



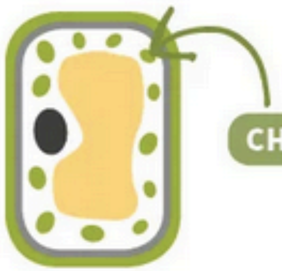
1. Molecule absorbs UV light
2. Loss of some energy (e.g. heat)
3. Energy released as visible light

When a UV light is shone on an egg shell it fluoresces bright red. This is due to the presence of protoporphyrin IX, which is a precursor of haemoglobin. It's also the compound which gives chicken eggs their brown colour.

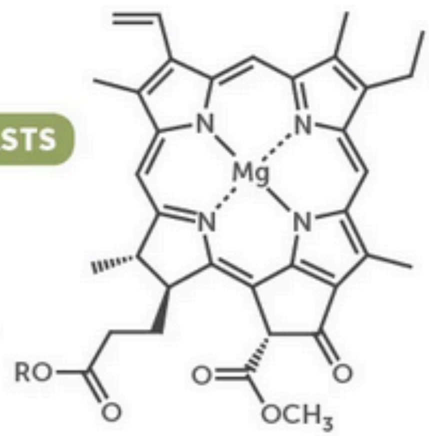
THE CHEMISTRY OF BROCCOLI

COOKING COLOUR CHANGES

Like other green vegetables, broccoli's colour comes from chlorophyll. Chlorophyll is found within the chloroplasts of plant cells. What causes this colour to intensify during cooking?



CHLOROPLASTS

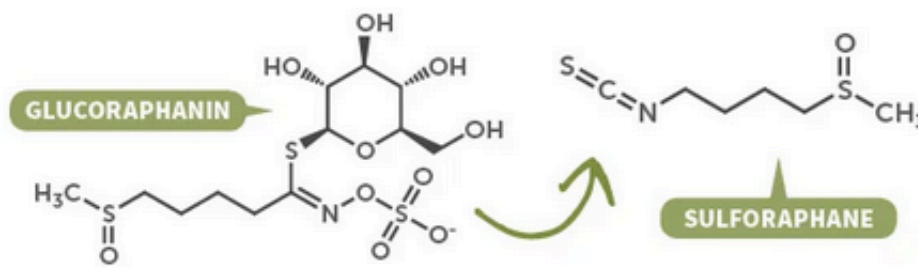


CHLOROPHYLL A

$R = C_{20}H_{39}$

Pockets of air in the space between plant cells cause the green of chlorophyll to be slightly clouded. During cooking these gas pockets expand and escape. This makes the green colour intensify. The effect doesn't last long, however. Cooking also causes plant cells to burst, releasing organic acids. Hydrogen ions from these acids react with chlorophyll to form pheophytins, making the greens less vibrant.

SULFORAPHANE AND CANCER



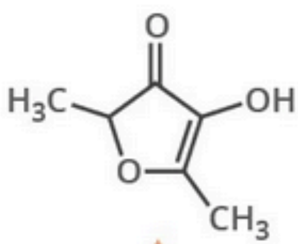
Chopping broccoli releases the enzyme myrosinase from cells. This acts on the glucosinolate compound glucoraphanin; one of the products is sulforaphane. Sulforaphane has been investigated due to its ability to kill cancerous cells. As myrosinase is heat-sensitive, cooking method affects the amount of sulforaphane present. Other sulfur compounds give broccoli its odour when cooked.

THE CHEMISTRY OF MANGOES

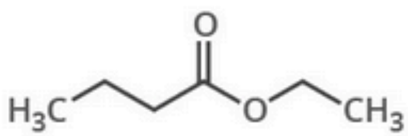
MANGO FLAVOUR & AROMA COMPOUNDS

A large number of compounds contribute to the flavour and the aroma of mangoes. The cultivar, maturity, and geographical origin of the mango all influence the compounds present.

270+ VOLATILE COMPOUNDS DETECTED IN MANGOES

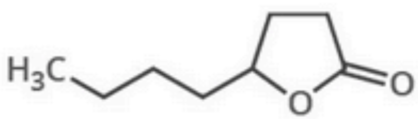


HDMF

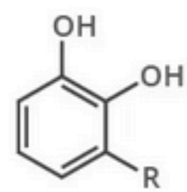


ETHYL BUTANOATE

γ-OCTALACTONE



MANGOES & CONTACT DERMATITIS



URUSHIOL

Possible R groups

$(CH_2)_{14}CH_3$

$(CH_2)_7CH{=}CH(CH_2)_5CH_3$

$(CH_2)_7CH{=}CHCH_2CH{=}CH(CH_2)_2CH_3$

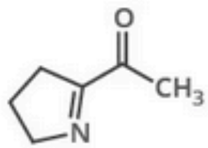
and others...

Esters such as ethyl butanoate account for fruity notes in mango aroma. A major contributor to sweet notes is HDMF (4-hydroxy-2,5-dimethyl-3(2H)-furanone). Lactones such as γ-octalactone can lend a coconut-like aroma, while terpenes are also found in significant quantities and make minor contributions.

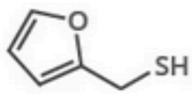
Mangoes belong to the same family of plants as poison ivy. Urushiol, a mix of similar organic compounds which are found in poison ivy and can cause a rash to develop on contact with the skin, can also be found in mango skin. This means that some people who are sensitive to urushiol get contact dermatitis when chopping or eating mangoes.

THE CHEMISTRY OF POPCORN

POPCORN FLAVOUR & AROMA COMPOUNDS

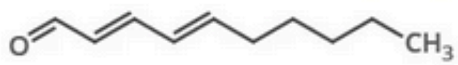


2-ACETYL-1-PYRROLINE

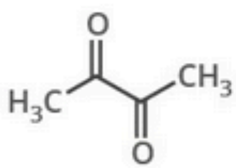


2-FURFURYLTHIOL

(E,E)-2,4-DECADIENAL

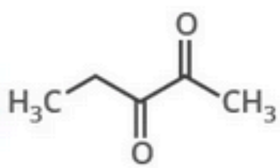


Many aroma compounds are given off by freshly prepared popcorn. Some of the most significant are 2-acetyl-1-pyrroline (which is a contributor to the roasty, popcorn-like aroma), (*E*,*E*)-2,4-decadienal (which has a fatty, fried aroma) and 2-furfurylthiol (which in isolation has a roasted coffee-like aroma). A range of other pyrazine, pyridine, and phenol compounds also contribute to flavour and aroma.



2,3-BUTANEDIONE

2,3-PENTANEDIONE



Flavourings added to popcorn can also contribute to the aroma. For example, butter-flavoured popcorn can include the compounds 2,3-butanedione (diacetyl) or 2,3-pentanedione. These compounds can cause respiratory problems in workers that inhale them while manufacturing the flavourings – the condition they can cause is known as 'popcorn lung'.

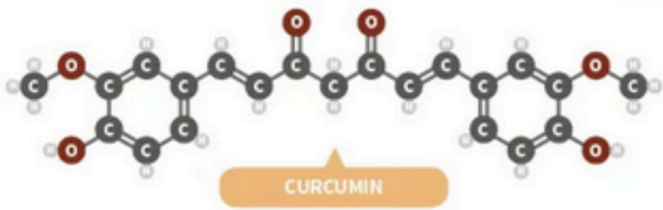
WHAT MAKES POPCORN POP?

The content of popcorn kernels is about 14% water. When the kernels are heated, this turns into water vapour at water's boiling point. However, it is trapped by the kernel's shell until the pressure builds up enough to crack through. The 'pop' is due to the escape of this pressurised water vapour, rather than the cracking of the kernel's shell. The molten starch bursts through the shell then rapidly cools, giving popcorn its fluffy appearance.

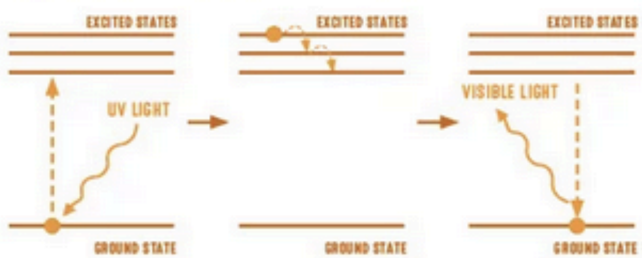
THE CHEMISTRY OF TURMERIC

Tumeric is a spice lauded for its supposed health benefits, and there are also some neat chemistry tricks you can do with it. Here we look at both!

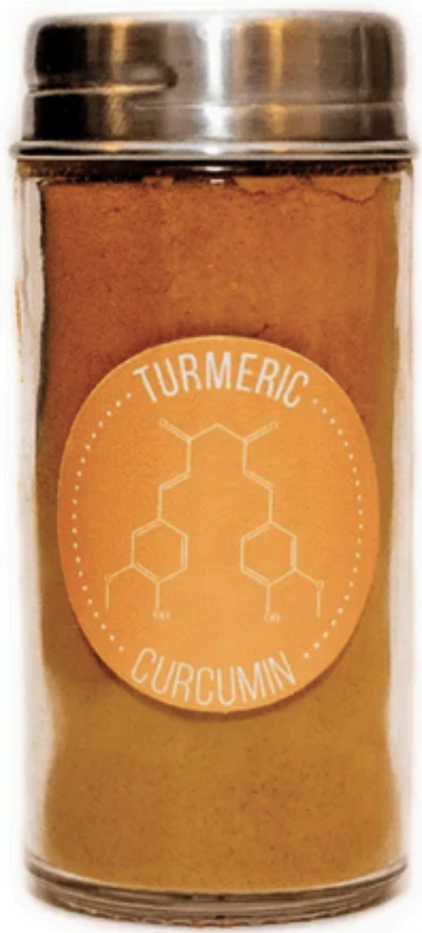
TURMERIC FLUORESCENCE



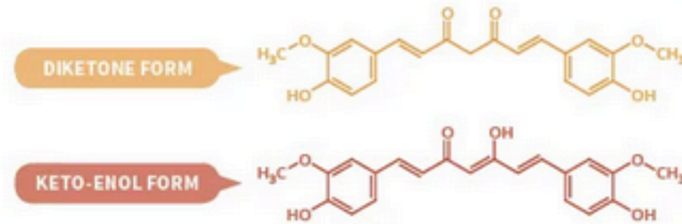
Curcumin is a key chemical component of turmeric, and can also make it fluoresce in the right conditions. If turmeric is sprinkled into alcohol whilst illuminated by UV light, a bright green-yellow fluorescence can be seen. Alcohol is used as curcumin is soluble in alcohol but not in water, and this helps make the fluorescence visible.



This fluorescence happens because the electrons in the curcumin molecules absorb the ultraviolet light, causing them to gain energy and move to an excited state. Some of the extra energy is lost as vibrational energy, and then the electrons fall back to the ground state, emitting visible light as they do so. This gives the green-yellow glow.



TURMERIC AS AN INDICATOR



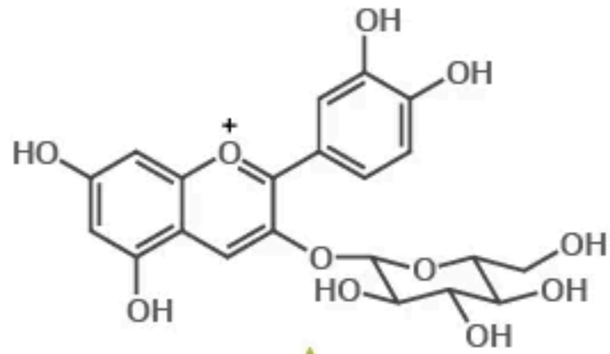
Curcumin's chemical structure is subtly different in acidic and alkaline solution. This allows it to be used as an indicator. When added to acids, it remains the yellow colour of turmeric. However, when added to an alkaline solution above pH 8, the shift of a hydrogen atom causes the compound to change colour, giving a red hue.

TURMERIC HEALTH BENEFITS

Anti-inflammatory, anti-oxidant and anti-cancer properties of curcumin have been observed in animal and laboratory studies. However, at present there have been too few clinical trials in humans to be able to confirm these effects. Curcumin is poorly absorbed and rapidly metabolised and eliminated when eaten, so little reaches our circulation.

BLACKBERRY CHEMISTRY

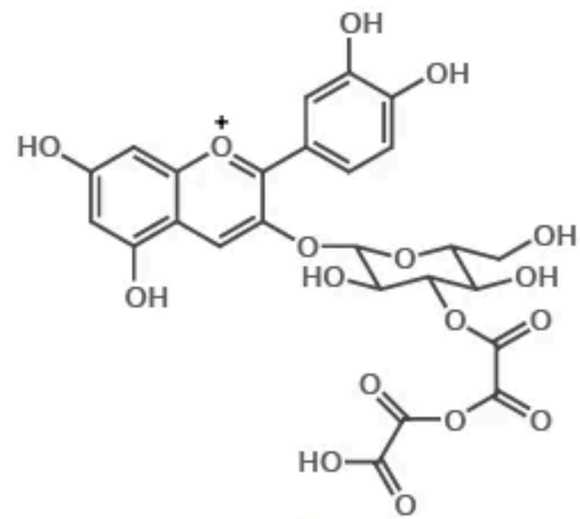
Summer may now be past its peak, but blackberry season is now fast approaching. In this graphic we briefly look at the compounds that give blackberries their purple-black colour.



CYANIDIN 3-GLUCOSIDE

Pigment compounds called anthocyanins give blackberries their purple to black colouration. They are a large group of pigments found in a number of other plants and flowers.

Cyanidin 3-Glucoside is the predominant anthocyanin in blackberries, but they also contain cyanidin 3-dioxalylglucoside, thought to be unique to blackberries.

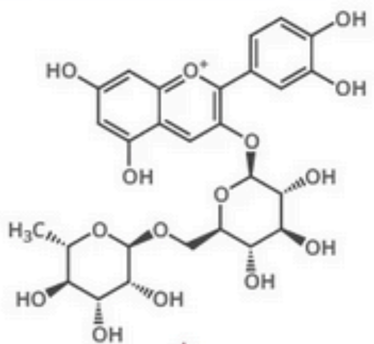


CYANIDIN 3-DIOXALYLGLUCOSIDE

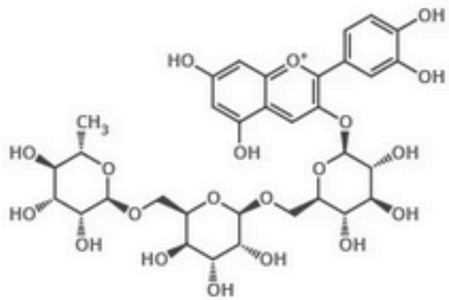
THE CHEMISTRY OF CHERRIES

Cherries are a popular summer fruit, and come in both sour and sweet varieties. Here we look at the chemical differences between the two.

SWEET CHERRIES AND SOUR CHERRIES

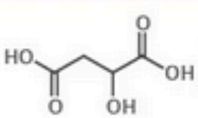


CYANIDIN-3-O-RUTINOSIDE



CYANIDIN-3-GLUCOSYLRUTINOSIDE

Cherry colour is due to the presence of compounds called anthocyanins. Sweet and sour cherries usually contain both of the compounds shown, but sweet cherries contain primarily cyanidin-3-o-rutinoside, whereas in sour cherries cyanidin-3-glucosylrutinoside is more abundant. Sour cherries also contain anthocyanins in greater concentrations.



MALIC ACID

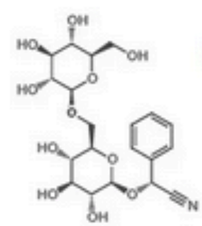
Sour cherries: 1.2–1.9%
Sweet cherries: 0.7–0.9%

Sour: pH 3.1-3.6

Sweet: pH 3.7-4.5

The tart flavour of sour cherries is due to the presence of a greater amount of malic acid. They have a titratable acidity of 1.2–1.9% of malic acid. Sour cherries also contain less sugar than sweet cherries.

POISONOUS PITS



AMYGDALIN

HYDROGEN CYANIDE

H—C≡N

BLACK CHERRY
~2.7mg/g

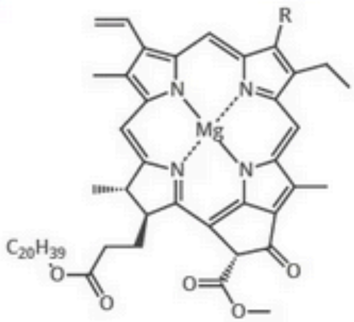
RED CHERRY
~3.9mg/g

Cyanogenic glycosides are found in the seeds of a number of fruits, including apples and apricots, and cherries are no exception. Their pits contain amygdalin, a compound which, when broken down during digestion, releases poisonous hydrogen cyanide. While a large number of the pits would need to be eaten by humans to see toxic effects, much less is needed for animals. Other parts of the cherry tree, including the leaves, are also toxic to animals.

THE CHEMISTRY OF BELL PEPPERS

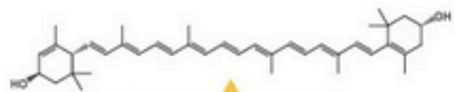
Bell peppers go through a spectrum of colours as they ripen – here we look at the compounds behind their colour, aroma, and flavour.

BELL PEPPER COLOUR CHEMISTRY

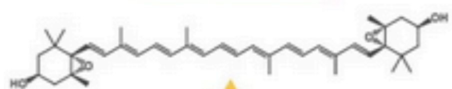


CHLOROPHYLL

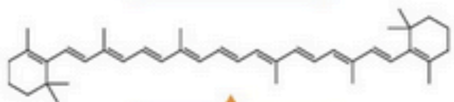
CHLOROPHYLL A: R = $-CH_3$
CHLOROPHYLL B: R = $-CHO$



LUTEIN

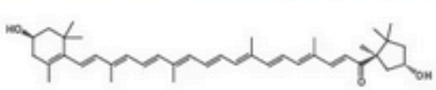


VIOLAXANTHIN

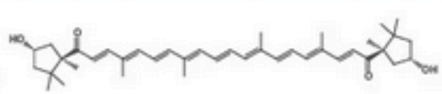


β-CAROTENE

Chlorophyll, used by plants for photosynthesis, gives bell peppers their initial green colour. As the pepper ripens, these are decomposed, and a range of carotenoid pigments appear. These include lutein, violaxanthin, and beta-carotene, which give yellow and orange hues. Eventually red carotenoid pigments including capsanthin and capsorubin appear. These red pigments are almost exclusively found in peppers.

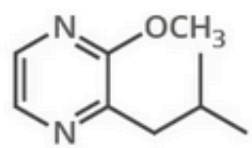


CAPSANTHIN

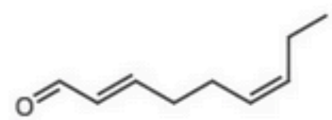


CAPSORUBIN

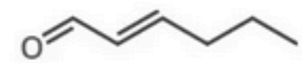
BELL PEPPER AROMA



BELL PEPPER PYRAZINE



CUCUMBER ALDEHYDE



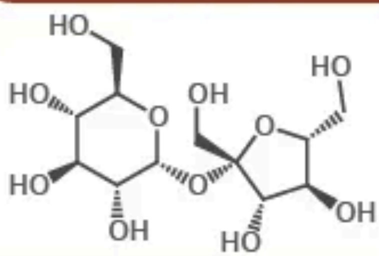
(E)-2-HEXENAL

The aroma of bell peppers also develops as they ripen. In green peppers, the characteristic smell is largely due to a single chemical, 2-methoxy-3-isobutylpyrazine ("bell pepper pyrazine"). Other minor contributors include (E,Z)-2,6-nonadienal ("cucumber aldehyde"). The concentrations of most volatile compounds drop during ripening, with the exception of (E)-2-hexenal and (E)-2-hexenol, lending a sweeter, fruitier note to the aroma.

MAPLE SYRUP CHEMISTRY

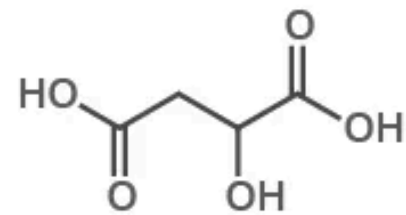
Maple syrup is the largest commercially produced product derived from tree sap. The sweet syrup has more constituents than just sugar, however. Here's a brief look at a small selection.

SUGARS



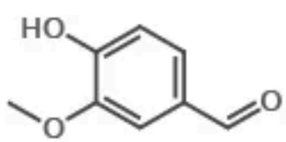
Sucrose is the main sugar in maple syrup, making up almost 70% of its composition. The percentages of other sugars are very low by comparison.

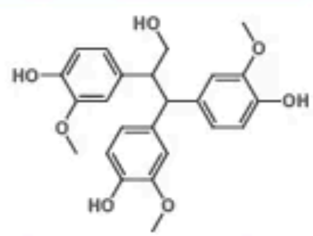
ACIDITY



Maple syrup is slightly acidic due to the presence of several organic acids. The most abundant of these is malic acid, at around 0.5%.

PHENOLIC COMPOUNDS

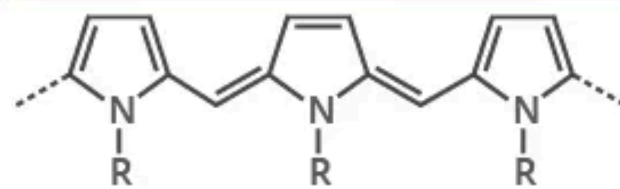




VANILLIN (ABOVE)
AND QUEBECOL (RIGHT)

Phenolic compounds in maple syrup form from degradation of lignin in sap, though some, like quebecol, form in the syrup-making process. Some contribute to the syrup's flavour, though the exact combination of compounds remains unclear.

SOURCE OF COLOUR



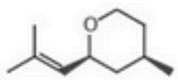
EXAMPLE FRAGMENT OF A MELANOIDIN STRUCTURE
(Melanoidins are brown polymers formed by the Maillard reaction)

Maple syrup is graded according to its colour. However, we still don't know the exact compounds behind its colouration. Maillard reactions, caramelisation, and formation of polycarbonyl compounds have all been implicated.

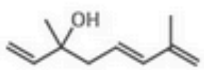
THE CHEMISTRY OF ELDERFLOWER & ELDERBERRIES

It's the time of year when elderflower bushes are bursting into bloom in the countryside. Here, we look at the chemistry of the flowers and the berries!

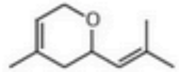
AROMAS OF ELDERFLOWER & ELDERBERRIES



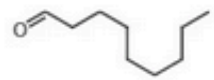
cis-ROSE OXIDE



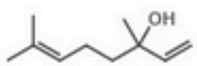
HOTRIENOL



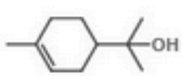
NEROL OXIDE



NONANAL

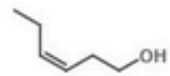


LINALOOL



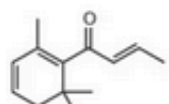
α-TERPINEOL

HEXANAL

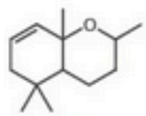


(Z)-3-HEXENOL

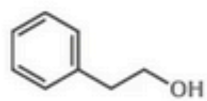
The compounds that make significant contributions to the aroma of elderflowers are *cis*-rose oxide, nerol oxide, hotrienol, and nonanal. Other compounds that contribute to the floral odour include linalool and α-terpineol, whereas hexanal and (Z)-3-hexenol add grassy odours.



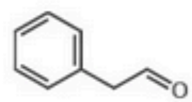
β-DAMASCENONE



DIHYDROEDULAN



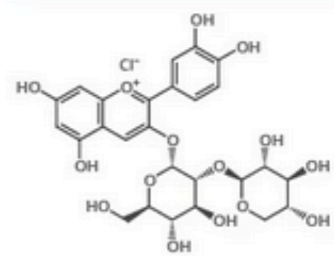
2-PHENYL ETHANOL



PHENYLACETALDEHYDE

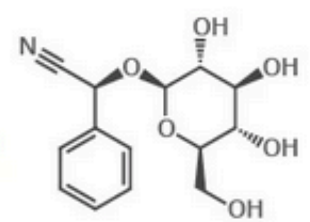
The key compounds that contribute towards the characteristic aroma of elderberries are β-damascenone and dihydroedulan, with 2-phenyl ethanol and phenylacetaldehyde also present. Several compounds present in the aroma of elderflowers also contribute, including linalool, and hotrienol.

ELDERBERRY COLOUR & TOXICITY



CYANIDIN 3-SAMBUBIOSIDE

SAMBUNIGRIN

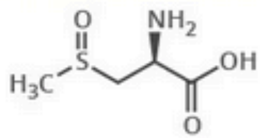


Coloured anthocynanins cause the colour of elderberries; the most abundant is cyanidin 3-sambubioside. Their high citric acid content contributes to their acidity. The leaves and stems of the plant, as well as elderberry seeds, contain moderate amounts of the cyanide-producing compound sambunigrin and the poisonous alkaloid sambucine. As such it's recommended that elderberries are always cooked before eating, as this breaks down these compounds.

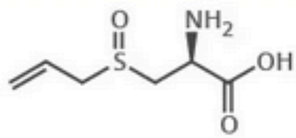
THE CHEMISTRY OF WILD GARLIC

Spring is in the air, and if you venture to a forest, so too is the smell of wild garlic. Here's a quick look at the chemistry of this common forest plant.

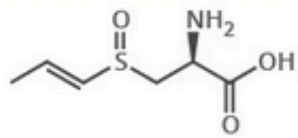
WILD GARLIC'S SMELL & COMPOSITION



METHIIN

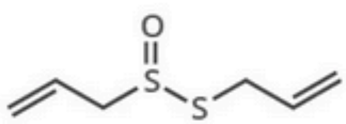


ALLIIN

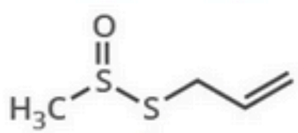


ISOALLIIN

The smell of wild garlic stems from the presence of sulfur-containing compounds called sulfoxides. Wild garlic contains a mix of methiin, alliin, and isoalliin. These compounds can be further broken down to give volatile thiosulfinate compounds, including allicin and methyl allyl thiosulfinate, as well as a range of others that contribute to the garlic odour.



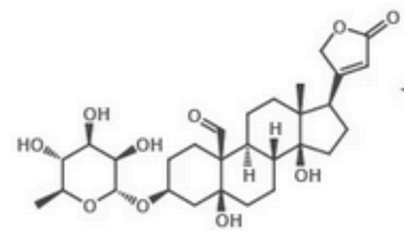
ALLICIN



METHYL-ALLYL THIOSULFINATE

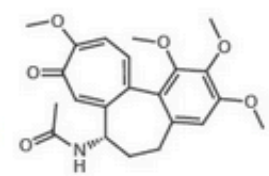
These breakdown compounds are produced by the plant as a consequence of mechanical damage. They serve an antimicrobial role; studies have shown that allicin shows inhibitory activity against both bacteria and fungi. Cows fed on wild garlic produce milk that tastes slightly of the plant as a consequence of some of the compounds present.

CASES OF MISTAKEN IDENTITY



CONVALLATOXIN

COLCHICINE



Other plants can be mistaken for wild garlic. These include lily of the valley, and the leaves of the autumn crocus. Lily of the valley contains a number of compounds known as cardiac glycosides, such as convallatoxin; autumn crocus leaves contain poisonous alkaloids (such as colchicine). Ingesting small amounts of either can lead to vomiting, diarrhoea, and even death. The leaves of both of these plants are devoid of wild garlic's characteristic smell.