The Last Frontier

Odors in the Indoor Environment

Alice Delia, PhD

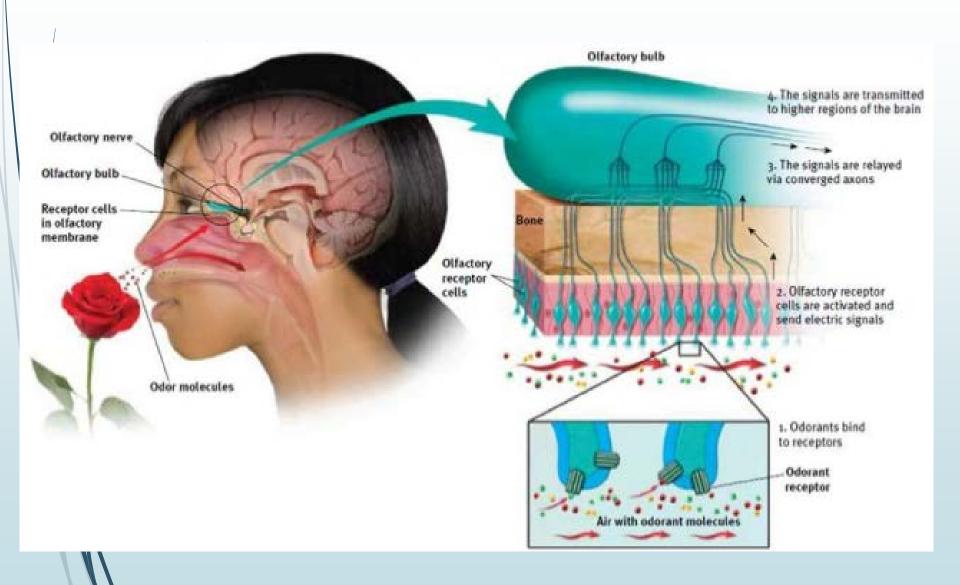
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An Odor Is ...



Understand

Explore

Identify

... the basics of volatile organic compounds (VOCs) and odors

... the world of odor characterization

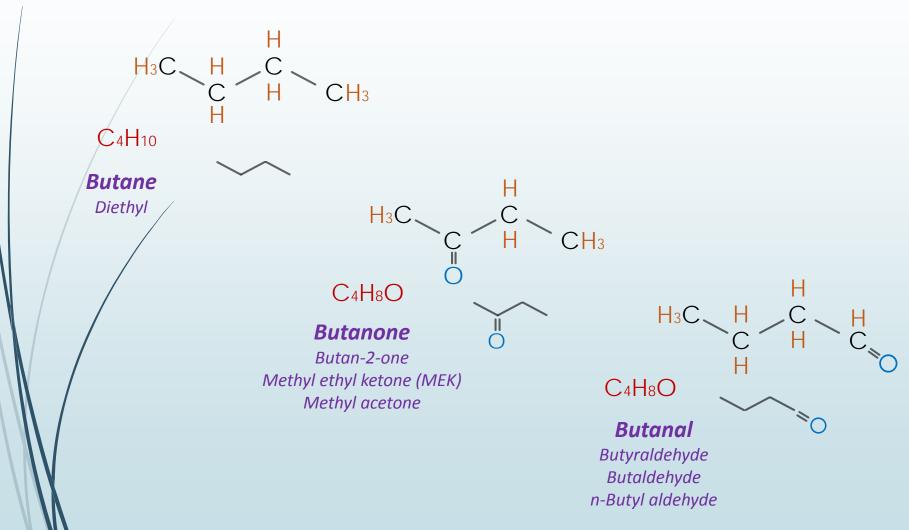
... odor sources based on chemical information

What is a VOC?

Volatile Organic Compounds

- Contains Carbon and Hydrogen
- Size: 6 16 Carbons
 OR
- ■Boiling Point: 50 250 °C

Functional Groups



FUNCTIONAL GROUPS IN ORGANIC CHEMISTRY

FUNCTIONAL GROUPS ARE GROUPS OF ATOMS IN ORGANIC MOLECULES THAT ARE RESPONSIBLE FOR THE CHARACTERISTIC CHEMICAL REACTIONS OF THOSE MOLECULES. IN THE GENERAL FORMULAE SHOWN BELOW FOR EACH FUNCTIONAL GROUP, 'R' REPRESENTS THE REST OF THE MOLECULE, AND 'X' REPRESENTS ANY HALOGEN ATOM.



SIMPLE OXYGEN HETEROATOMICS



HALOGEN HETEROATOMICS



CARBONYL COMPOUNDS



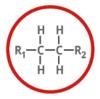
NITROGEN-BASED



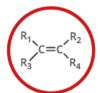
SULFUR-BASED



AROMATIC



ALKANE Naming: -ane e.g. ethane



ALKENE Naming: -ene e.g. ethene



ALKYNE Naming: -yne e.g. ethyne



ALCOHOL Naming: -ol e.g. ethanol



ETHER Naming: -oxy -ane e.g. methoxyethane



EPOXIDE Naming: -ene oxide e.g. ethene oxide



HALOALKANE Naming: haloe.g. chloroethane



ALDEHYDE Naming: -al e.g. ethanal



AMINE Naming: -amine e.g. ethanamine



KETONE

Naming: -one

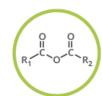
NITRILE Naming: -nitrile e.g. ethanenitrile



CARBOXYLIC ACID Naming: -oic acid e.g. ethanoic acid



IMINE Naming: -imine e.g. ethanimine



ACID ANHYDRIDE Naming: -oic anhydride e.g. ethanoic anhydride



ISOCYANATE Naming: -yl isocyanate e.g. ethyl isocyanate



ESTER Naming: -yl -oate e.g. ethyl ethanoate



AZO COMPOUND Naming: azoe.g. azoethane



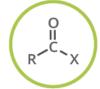
AMIDE Naming: -amide e.g. ethanamide

R-SH

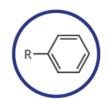
THIOL

Naming: -thiol

e.g. methanethiol



ACYL HALIDE Naming: -oyl halide e.g. ethanovl chloride



ARENE Naming: -yl benzene e.g. ethyl benzene





Odor Sources



Animals



Plants

Food



Furniture







Trash

50% of ...

Detection

Detect Odor without characterizing it

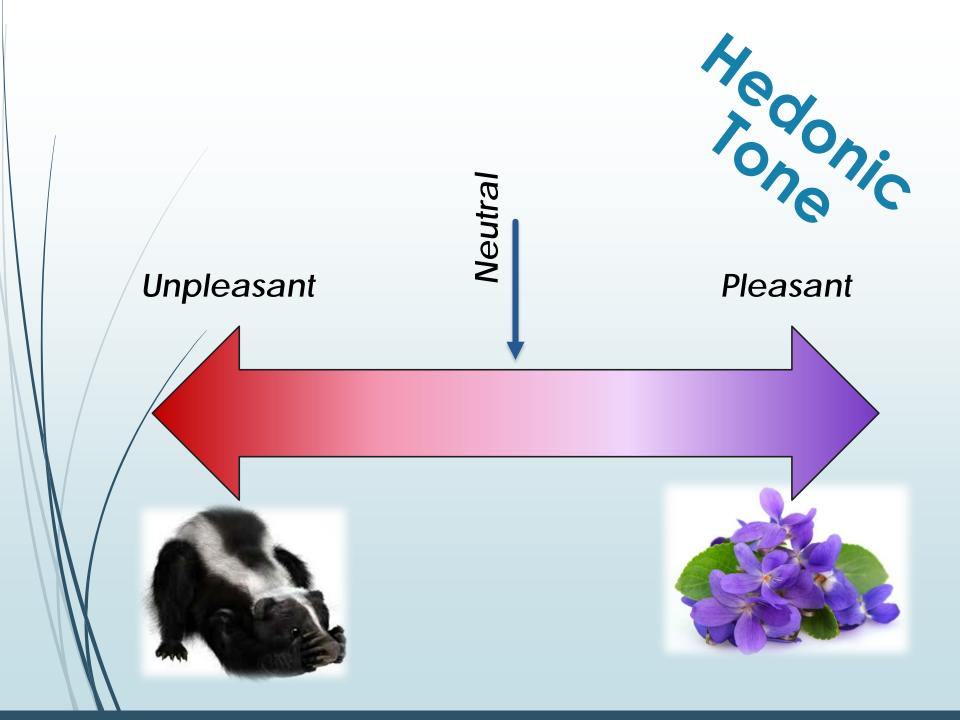
Odor

Respond to Odor

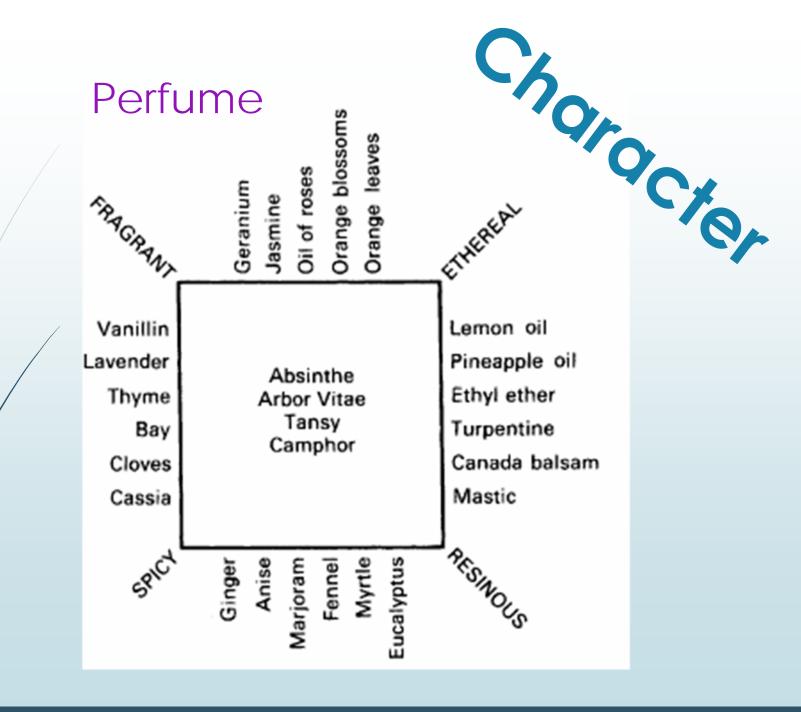
Recognition

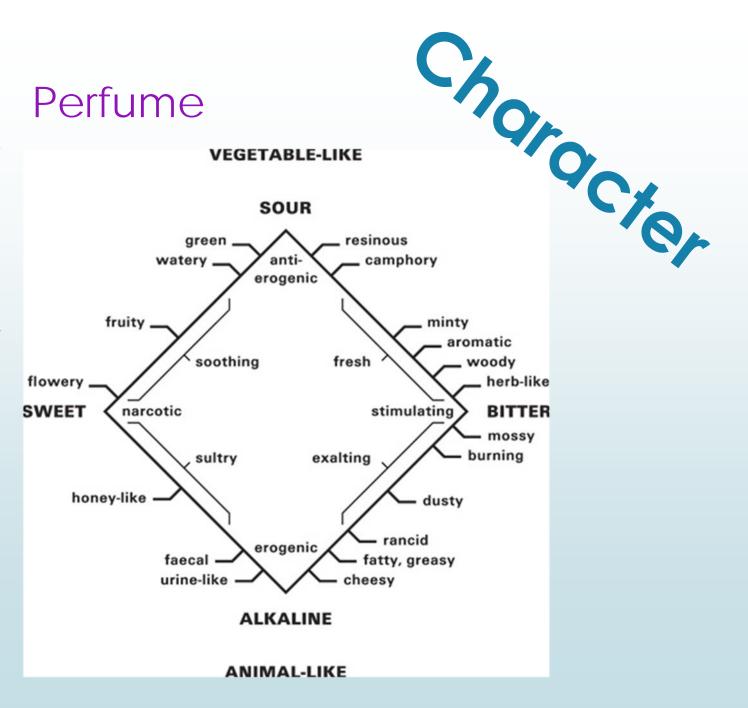
Identify Specific Odor

- 0 No Odor
- 1 Very Weak(Threshold)
- 2 Weak
- 3 Distinct
- 4 Strong
- 5 Very Strong
- 6 Intolerable



Fruity Henning Flowery Putrid Spicy Resinous Burnt





centration ppb)	Character	Compound
9 *		Sulfur dioxide
0.47	Rotten eggs	Hydrogen sulfide
210	Sulfide	Carbon disulfide
210	Green/sweet	Acetaldehyde
1000	Pungent	Formaldehyde
2.1	Pungent	Methyl mercaptan
47	Medicinal	Phenol
0.21	Fishy, pungent	Trimethyl amine
210	Burnt sweet	Acrolein

^{*} All concentrations are in parts per billion (ppb) G. Leonardos (Odor Threshold Determinations of 53 Odorant Chemicals)



Odor vs Chemical

- Odors are perception of the physiological process
- Chemicals (VOCs) are what starts that process
- Odors and physical symptoms are both effects
- Odor compound may or may not be responsible for physical symptoms; there is no specific relationship linking the odor to other effects

What Causes Release of Chemicals

Damage

- Cut
- Decomposition/decay/death

Chemical conversion (e.g., photosynthesis, plant respiration)

Stress

Attract or Repel

■ Pheromones

Organic ChemistryTable of organic compounds and their smells

Ĭ	ALKANES AL		ALKENES	ALCO	HOLS	ALDEHYDES			KETO	ONES	CARBOXY	LIC ACIDS	HALOALKANES			THIOLS	THIOLS AMINES		NITRILES	LACTONES	
9.0	-ane	cyclo -ane	-ene	-anol	-an-2-ol	-anal	2-methyl -anal	3-(4-r-butylphenyl) -anal	-enal	-an-2-one	methyl -an-2-one	-anoic acid	-enoic acid	chloro -ane	bromo -ane	iodo -ane	-anethiol	-anamine	diamino -ane	-anenitrile	-anolide
meth- 1 carbon	none	doesn't exist	carbene is too unstable to smell	ABSOLUT	doesn't exist	FORMALDEHYDE INSTANT ACTIONS PRODUCED IN ACTION ACTIONS ACTIONALLY PRODUCED IN ACTION	doesn't exist	doesn't exist	doesn't exist	doesn't exist	doesn't exist	PUNGENT & PENETRATING	doesn't exist	TOXIC & MILDLY SWEET	LIKE	SWEET, ACRID	10		?		doesn't exist
eth- 2 carbons	none	doesn't exist	000	ABSOLUT VODKA	doesn't exist	FRUITY, ETHEREAL	doesn't exist	doesn't exist	doesn't exist	doesn't exist	doesn't exist	VINEGAR	doesn't exist	MILDLY	SWEET, ACRID	ETHEREAL	SKUNK			ETHEREAL	doesn't exist
prop -3 carbons	none	- D	00	ABSOLUT VODKA	RUBBING ALCOHOL	IRRITATING GREEN COFFEE	WET	ATTRACTS SPERM	BURNED GREASE	NAIL VARNISH REMOVER	doesn't exist	SLIGHTLY	SHARP	MILDLY	SWEET	SHARP, UNIQUE	1			ETHEREAL	none
but - 4 carbons	none				godds.	PUNGENT BANANA	1	LILY	PUNGENT & SUFFOCATING	BUTTERSCOTCH	LIKE NAIL VARNISH REMOVER	RANCID BUTTER	BROWN	SHARP	PLEASANT, SWEET	SHARP, UNIQUE	butanethiel skunk 2-methyl butan-2-thiel natural gas odorart		DEAD-	SUFFOCATING	
pent- 5 carbons	STARTING FLUID	PLEASANT	6	STRONG SWEET	(S)- and (R)- enantiomers	PUNGENT NUTS & CHOCOLATE	FRESHLY CUT GRASS	?		4	MINT (4-methyl-)	DISGUSTING		MILD	PLEASANT, SWEET	1	ROASTED		DEAD ANIMALS & URINE		HERBAL
hex- 6 carbons	STARTING FLUID	SWEET	600	FRESHLY CUT GRASS	-	FRESHLY CUT GRASS	FRESHLY CUT GRASS	?	J	ATTRACTS	(3-methyl-)	GOATS	ARMPITS (WHEN 3- METHYLATED)	AROMATIC	SLIGHTLY SWEET	?	BURNED		ROTTING FISH		
benzene different naming system is used	n/a	n/a	Benzene	SICKENINGLY SWEET AND TARRY Phenol	doesn't exist	W.	***	?	doesn't exist	doesn't exist	Acetophenone	BALSAMIC	doesn't exist	The state of the s	AROMATIC		W • •	Aniline	TOXIC, AROMATIC	Benzonitrile	doesn't exist
hept- 7 carbons			600	FRESHLY CUT GRASS	(S)- and (R)- enantiomers	STRONG, FRUITY COGNAC	(2,6-dimethyl- heptanal)	?	ALMOND BUTTER	4	BAD (6-methyl-)	RANCID	ARMPITS (WHEN 3- METHYLATED)	none	SLIGHTLY SWEET	none	1 € €				CARAMEL &
oct- 8 carbons	PETROL		- O	PENETRATING, SWEET	(S)- and (R)- enantiomers	STRONG, CITRUS- LIKE	?	?		-2-one petrol -3-one herb butter	?	M. Comments	ARMPITS	none	0	SEAWEED	STENCH		H		
non- 9 carbons	DIESEL	•	O	CITRUS	%	ATTRACTS MOSQUITOES		?	OLD PEOPLE	MILK	?	RANCID	ARMPITS	none	none	none	OBNOXIOUS			\triangle	
dec- 10 carbons	JET FUEL		O	CITRUS FLOWERS	?	BUCKWHEAT		?	ATORA TALLOW	?	?	M	ARMPITS	none	none	none	OBNOXIOUS				
undec- 11 carbons	ALSO ANT 'PANIC' PHEROMONE	?	O	CITRUS FLOWERS	?	MAKES SPERM UNABLE TO FIND THE EGG	KUMQUATS	?	a.	ALGERIAN OIL OF RUE	?	WAXY	PUNGENT & PENETRATING	UNIQUE & UNPLEASANT	none	MOUSE PHEROMONE	OBNOXIOUS			\triangle	
dodec- 12 carbons	- D	MUSTY,	O	FLOWERS	?		?	?	4 🖸	?	?	BAY OIL	FATTY	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS	9			
tridec- 13 carbons	STINK-BUG PHEROMONE	UNIQUE; FOUND IN ROSES	- D	PLEASANT	?	GRAPEFRUIT PEEL	ROASTED	?	?	WAXY	?		?	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS		none	\triangle	ANGELICA ROOT
tetradec- 14 carbons	KAPOK BUSH FLOWERS	none	- D		?		?	?	?	?	?	WAX & NUTMEG	?	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS		none		CEDAR
pentadec- 15 carbons	TAMARIND (ANT-CALMING PHEROMONE)	?	- N		?	FRESH	?	?	CORIANDER	CELERY	?	BIOMARKER FOR DAIRY CONSUMPTION (No smell)	?	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS		none	\triangle	MUSK

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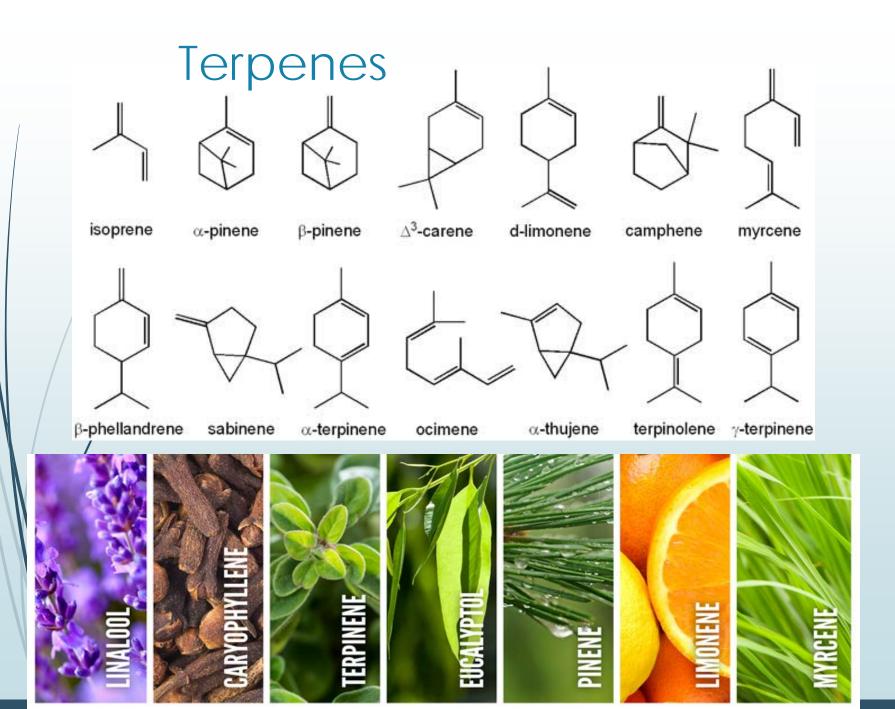
from the carboxylic acid (second word)

from the alcohol (first word)

				mom un	e alconor (ilist word	,				
	methyl 1 carbon	ethyl 2 carbons	propyl 3 carbons	2-methyl propyl-	butyl 4 carbons	pentyl 5 carbons	hexyl 6 carbons	benzyl benzene ring	heptyl 7 carbons	octyl 8 carbons	nonyl 9 carbons
methanoate 1 carbon	ETHEREAL	BACARDÍ		ETHEREAL	*		"GREEN"	100			?
ethanoate 2 carbons	BI III	· All			6			JASMINE		6	1
propanoate 3 carbons			A L							6	?
2-methyl propanoate 4 carbons, branched		ETHEREAL	BACARDÍ				HANN				?
butanoate 4 carbons			00			10	0			and the same	?
pentanoate 5 carbons				A L	ETHEREAL			N	-	?	?
hexanoate 6 carbons				N			*				
benzoate benzene ring	YLANG YLANG	H	NUTS	BALSAMIC						?	1
heptanoate 7 carbons				-	©	?	-	A.	-	60	?
salicylate from salicylic acid	8 0		MINT	WINTERGREEN	THONG		rwal i Jan	DIFFERENT PEOPLE PERCEIVE DIFFERENT AROMASI	?		?
octanoate 8 carbons	0		0			CO:				S	0
phenylacetate benzene ring + 2 carbons	STRONG		1000		-	2		JASMINE	none!		?
nonanoate 9 carbons	So T			0						?	
cinnamate benzene ring + propenol		76							Ţ		?
decanoate 10 carbons			OIL S	1	Mr Dina	-	?	?	?	?	?

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Ethyl heptanoate	~~lo	apricot, cherry, grape, raspberry			Cotoro				
Ethyl isovalerate	Lin	apple			Esters				
Ethyl lactate	~° → OH	butter, cream	Methyl salicylate (oil of wintergreen)	CY _{OH}	Modern root beer, wintergreen, Germolene and Ralgex ointments (UK)				
Ethyl nonanoate	~~~h	grape	Nonyl caprylate	~~~	orange				
Ethyl pentanoate	~lo~	apple	Octyl acetate	l	fruity-orange				
Geranyl acetate	المحلما	geranium	Octyl butyrate	مام	parsnip				
Geranyl butyrate	Lille	cherry	Amyl acetate (pentyl acetate)	i.~~	apple, banana				
Geranyl pentanoate	سلسل	apple	Pentyl butyrate (amyl butyrate)	٠١٠٠٠	apricot, pear, pineapple				
Isobutyl acetate	ئہ	cherry, raspberry, strawberry	Pentyl hexanoate (amyl caproate)	~~l~~	apple, pineapple				
Dutyl acciaic	X 0,	apple, noticy	Pentyl pentanoate (amyl valerate)	سأس	apple				
Butyl butyrate Isoamyl acetate	ا ا	pineapple pear, banana (flavoring in Pear drops)	Propyl acetate	· ^ Å	pear				
Isopropyl acetate	i,	fruity	Methyl anthranilate	CT _{NH2}	grape, jasmine				
Linalyl acetate	**************************************	lavender, sage	Methyl benzoate	O'	fruity, ylang ylang, feijoa				
Linalyl butyrate		peach	Methyl butyrate (methyl butanoate)	مأه	pineapple, apple, strawberry				
Linalyl formate		apple, peach	Methyl cinnamate	ON	strawberry				
Methyl acetate		glue	Methyl pentanoate (methyl valerate)	~\lo	flowery				
	<i>></i> 0		Methyl phenylacetate	Qi	honey				
Methyl anthranilate	CV _{NH2}	grape, jasmine	Methyl salicylate (oil of wintergreen)	CY _{OH}	Modern root beer, wintergreen, Germolene and Ralgex ointments (UK)				
Methyl benzoate	مأه	fruity, ylang ylang, feijoa	Nonyl caprylate	~~!~~~	orange				
		3, 3, 4,	Octyl acetate	المحمد	fruity-orange				
Methyl butyrate (methyl butanoate)	a l	pineapple, apple, strawberry	Octyl butyrate	مأسسا	parsnip				
Methyl cinnamate	~ l	strawberry	Amyl acetate (pentyl acetate)	ئىرى	apple, banana				
T Shirt and			Pentyl butyrate (amyl butyrate)	~å~~	apricot, pear, pineapple				
Methyl pentanoate (methyl valerate)	~~~~°	flowery	Pentyl hexanoate (amyl caproate)	~~l~~	apple, pineapple				
Methyl phenylacetate	() i	honey	Pentyl pentanoate (amyl valerate)	~l~~	apple				
	0	· · · · · · · · · · · · · · · · · · ·	Propyl acetate		pear				
			Propyl hexanoate	~\ildot	blackberry, pineapple, cheese, wine				



Odor Chemistry - Seaside

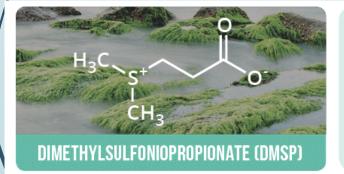


The characteristic smell of the seaside stems from volatile organic compounds that contain sulfur. Some of these compounds are emitted by algae in the sea, as a result of enzymatic activity or bacterial action, whilst others can be emitted by decomposing seaweed on the beach itself.

COMPOUNDS FROM BACTERIA

Hydrogen sulfide gas is produced by decomposing seaweed; the anaerobic breakdown of sulfates in the seaweed leads to the production of the gas. It is toxic in high concentrations, but as it is produced naturally in the body, humans have mechanisms to break it down, so can tolerate low concentrations.

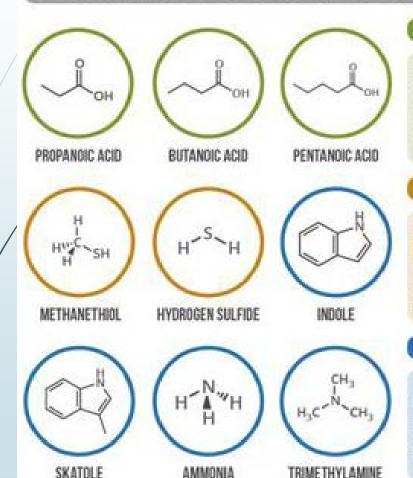




Dimethylsulfoniopropionate (DMSP) is a compound found in algae cells, which acts as an osmolyte (maintains cell volume and water levels). This compound can be broken down by both enzymes and bacteria, and this can produce dimethylsulfide (DMS). DMS is considered a major component of the smell of the sea.

Odor Chemistry - Waste

A SELECTION OF ODOUR COMPOUNDS FROM HUMAN WASTE



FATTY ACIDS

Fatty acids in faeces contribute a number of unpleasant odours. The most common is ethanoic (acetic) acid, but the longer chain length acids are bigger odour contributors. Butanoic (butyric) acid is one of these, and is also in part responsible for the smell of vomit. Both it and pentanoic (valeric) acid have putrid, rancid smells in isolation.

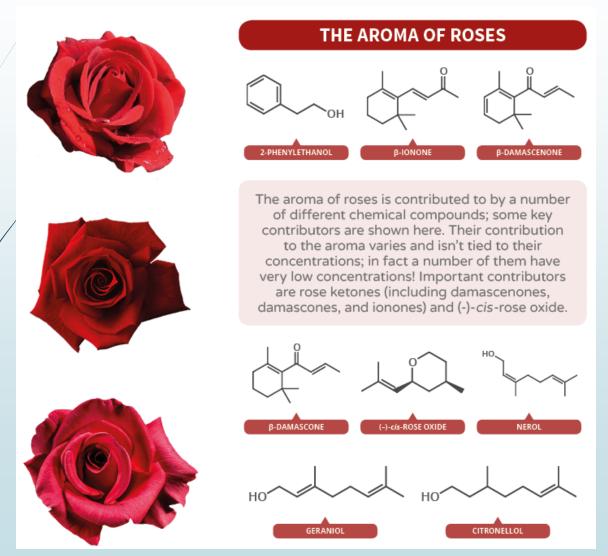
SULFUR-CONTAINING

Sulfur-containing compounds are the main odourants of human faeces. Chief amongst these are hydrogen sulfide, the odour of which is often described as akin to rotting eggs, and methanethiol, whose odour is described as eggy and onion-like. Both have low odour thresholds, meaning even at low concentrations they have significant impact.

NITROGEN-CONTAINING

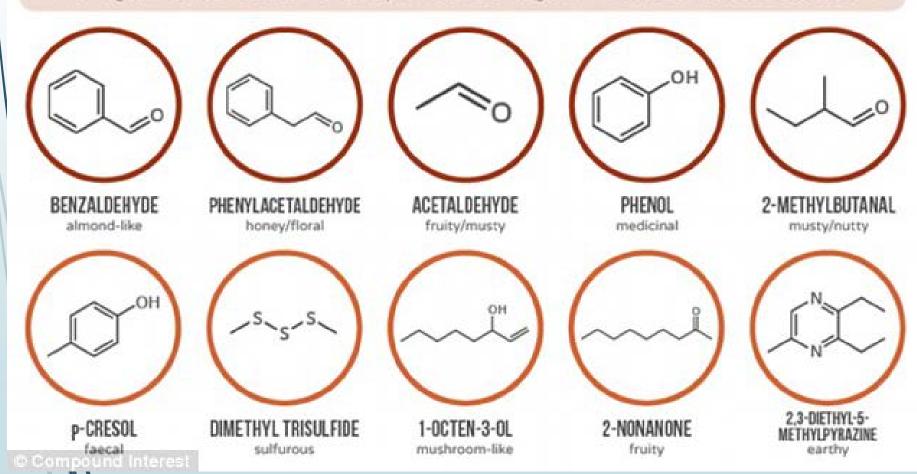
Indole and skatole are both constituents of faeces, and both have a faecal, animal odour. However, at low concentrations, their aroma is pleasant and floral, and they are found in some flowers. Ammonia and trimethylamine are produced by breakdown of urea in urine; the odour threshold for trimethylamine is much lower than that for ammonia.

Odor Chemistry – Roses



Odor Chemistry - Wet Dog

The smell of dogs is complex: multiple chemical compounds contribute which individually do not have odours associated with dog smell, but produce it in combination. A pilot study found emitted concentrations of some compounds increased when dog hair was wet. Those shown on the top row below showed greater increases than those on the second row.



Good Smells vs Bad Smells



Understand

Explore

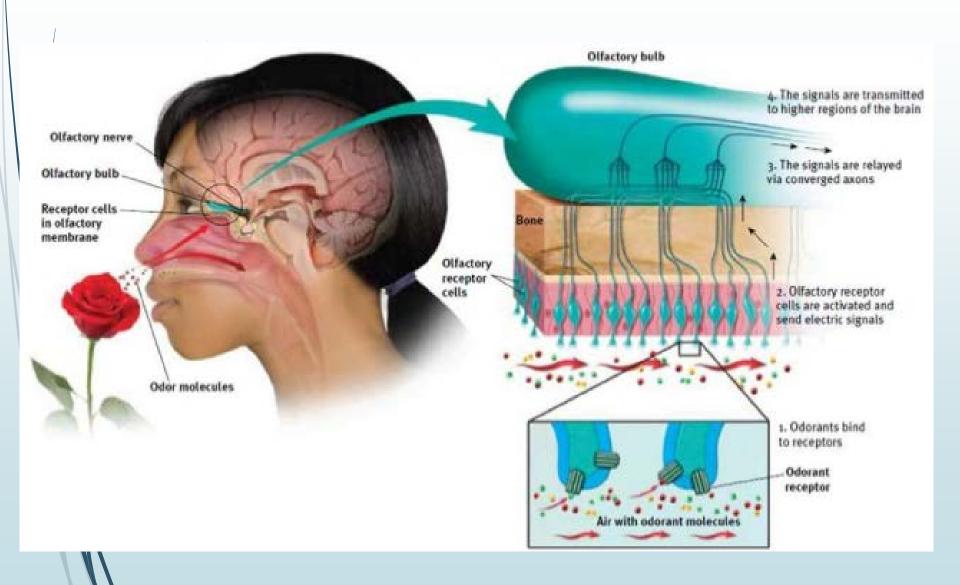
Identify

... the basics of volatile organic compounds (VOCs) and odors

... the world of odor characterization and measurement

... odor sources based on chemical information

Sense of Smell



Facets

- **■**Sources
- **■**Thresholds
- Intensity
- ■Tone
- Character

VOCs

- C and H
- Volatility
 - **■**Temperature
 - Humidity
- Functional Groups
 - **■**Specific Order

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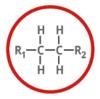
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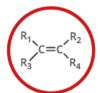
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EPOXIDE Naming: -ene oxide e.g. ethene oxide



HALOALKANE Naming: haloe.g. chloroethane



ALDEHYDE Naming: -al e.g. ethanal



AMINE Naming: -amine e.g. ethanamine



KETONE

Naming: -one

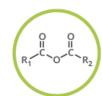
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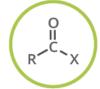
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R-SH

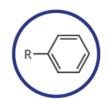
THIOL

Naming: -thiol

e.g. methanethiol



ACYL HALIDE Naming: -oyl halide e.g. ethanovl chloride



ARENE Naming: -yl benzene e.g. ethyl benzene





Terms

Odorant – substance capable of eliciting an olfactory response Odor – sensation resulting from stimulation of the olfactory organs

Detection Threshold – 50% can identify presence of odor or odorant without characterizing it (smell something but can't say what it is)

Odor Threshold – concentration at which 50% of the individuals exposed to the odorant respond

Recognition Threshold - 50% identify odorant or odor

Odor Adaptation – process by which one becomes accustomed to odor

Odor Fatigue – total adaptation occurred through prolonged exposure

Odor Tenacity - persistence; time odor remains perceptible

References

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- Gregory Leonardos, David Kendall & Nancy Barnard; Odor Threshold Determinations of 53 Odorant Chemicals, J Air Pollution Control Assn, 19:2, 91-95, 1969.
- J.H. Ruth, Odor Thresholds and Irritation Levels of Several Chemical Substances: A Review, 1986.