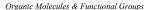
# Organic Molecules Structures, Functional Groups, Reactions

Dr. Ron Rusay



## Functional Groups & Amino Acids



The following simple molecules: water, ammonia, methane, formaldehyde and formic acid can be used as "lego-like" building blocks to construct the vast majority of organic and biological molecules. Simply replace a hydrogen from each of any two molecules with a bond to the central atom, and if joining three molecules replace 4 hydrogens with 2 bonds.

water	ammonia	methane	formaldehyde	formic acid
0	3		•••	

Name	General Formul

Alcohols R-OH

Ethers R-O-R'

Amines R-NH<sub>2</sub>

Carboxylic Acids R-C-OH

Aldehydes

R-C-H

Ketones

Q
R-C-R'

Carboxylic Acids

R-C-R'

Q

R-C-OH

Esters
Q
R-C-OF
Amides
Q
R - C - OF

Chem 108 / Dr. Rusay

#### 20 Amino Acids found in Proteins of Living Organisms

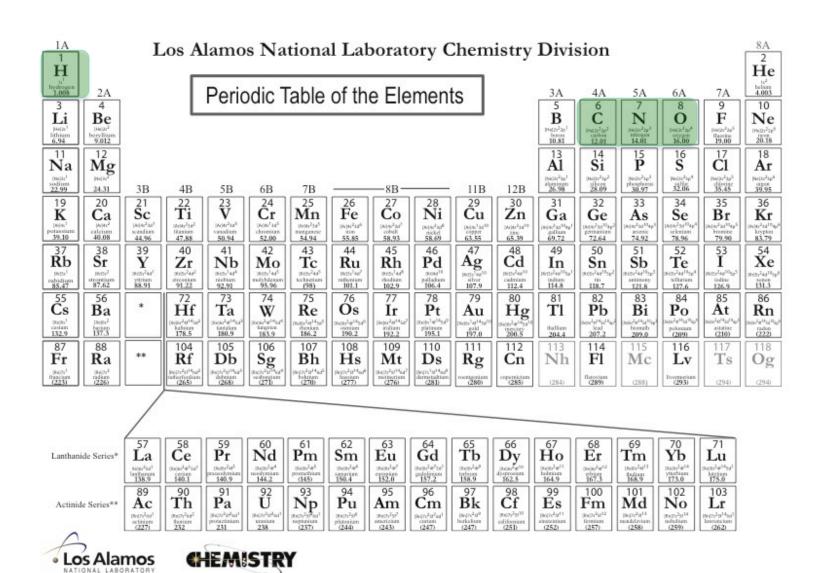




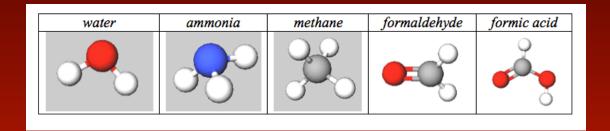
#### https://chem.libretexts.org/LibreTexts/Diablo\_Valley\_College/DVC\_Chem\_106%3A\_Rusay/Amino\_Acids

Name	I	II	R-	R'-	Rasmol Color	Function & Class	
Alanine	Ala	A	H-	CH <sub>3</sub> -	dark gray	Aliphatic Hydrophobic	
Arginine	Arg	R	H-	-CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NHCNH <sub>2</sub>	blue	Basic Hydrophilic	
Asparagine	Asn	N	H-	O    -CH <sub>2</sub> CNH <sub>2</sub>	cyan	Amide Highly Hydrophilic	
Aspartate	Asp	D	H-	O    -CH <sub>2</sub> COH	bright red	Acidic Hydrophilic	
Cysteine	Cys	С	H-	-CH <sub>2</sub> SH	yellow	Sulphur Containing Hydrophobic	
Glutamine	Gln	Q	H-	O    -CH <sub>2</sub> CH <sub>2</sub> CNH <sub>2</sub>	cyan	Amide Highly Hydrophilic	
Glutamate	Glu	Е	H-	-CH <sub>2</sub> CH <sub>2</sub> COH	bright red	Acidic Hydrophilic	
Glycine	Gly	G	H-	H-	light gray	Aliphatic Hydrophobic	
Histidine	His	Н	H-	H CH <sub>2</sub> -	pale blue	Basic Hydrophilic	
Isoleucine	Ile	I	H-	CH <sub>3</sub> -CHCH <sub>2</sub> CH <sub>3</sub>	green	Aliphatic Hydrophobic	
Leucine	Leu	L	H-	CH <sub>3</sub> -CH <sub>2</sub> CHCH <sub>3</sub>	green	Aliphatic Hydrophobic	

### Elemental building blocks for all organic molecules



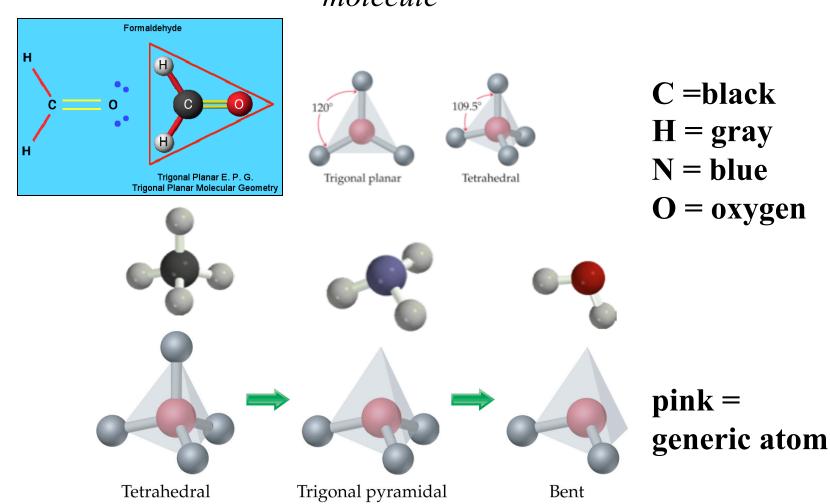
## Organic Molecules



Shapes, Functions & Structural Analogies Water, Ammonia, Methane

## Molecular Models for C, H, N, O

Fundamental repeating shapes found in every biological molecule



## Representing Organic Molecules



http://chemconnections.org/general/movies/Representations.MOV

## Representing Organic Molecules Common Formulas & Drawings

Molecular formula:  $C_7H_{16}O$  Empirical Formula:  $C_7H_{16}O$ 

#### **Condensed Structure:**

CH<sub>3</sub>CH<sub>2</sub>C(CH<sub>3</sub>)<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OH or CH<sub>3</sub>CH<sub>2</sub>CCH<sub>2</sub>CH<sub>2</sub>OH

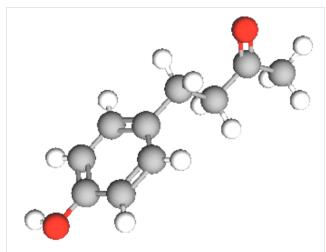
 $CH_3$ 

 $CH_3$ 

**Bond-Line Structure:** 

A compound that smells like fresh raspberries, the following structure, C<sub>?</sub>H<sub>?</sub>O<sub>?</sub>, matches its calculated molar mass which is 164 g/mol.

- A) TRUE
- B) FALSE





## **Organic Molecules**

#### Common Functional Groups

### Name

### General Formula

Alcohols

represents any

R'- or R-

R-OH

**Ethers** 

generic carbon atom bonded in the functional

R-O-R'

**Amines** 

group

R-NH<sub>2</sub>

R-C-OH

### Carboxylic Acids

water	ammonia	methane	formaldehyde	formic acid
	3			

## **Organic Molecules**

#### Common Functional Groups

### **Name**

#### **General Formula**

### **Aldehydes**

#### **Ketones**

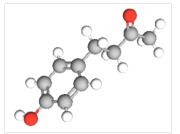
## **Carboxylic Acids**

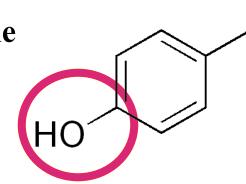
**Esters** 

**Amides** 

R'- or Rrepresents any
generic carbon
atom bonded in
the functional
group

Select the function(s) in the molecule



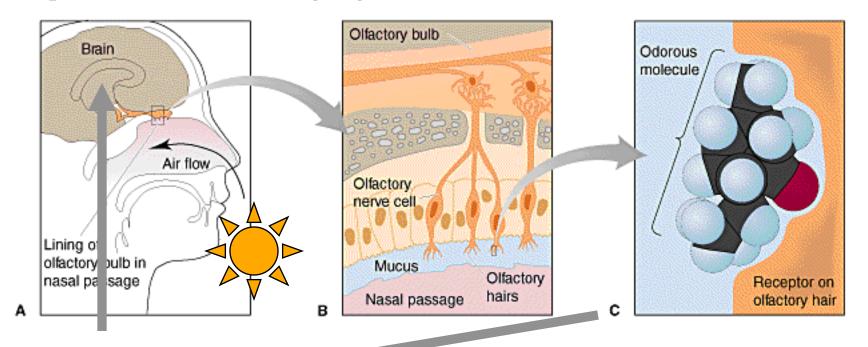


Alcohol R-OH Ether R-O-R' Amine R-NH <sub>2</sub>
Amine R-NH <sub>2</sub>
Aldehyde O R-C-H
Ketone R-C-R'
Carboxylic Acid OR-C-OH
Ester $R$ -C-OR' $Q$ $R$ '
Amide R-C-N



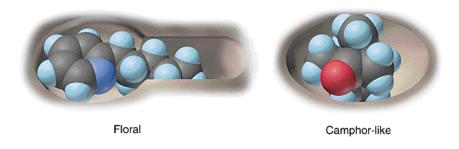
## Detecting stuff we cannot see: the Sense of Smell Models, Theories & Interactions

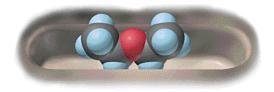
http://chemconnections.org/organic/chem226/Labs/Smell/smell-links.html



Structure-Odor Relationships Karen J. Rossiter, Chem. Rev., 1996, 96, 3201-3240

#### Historical view of a few smell receptors.





#### **4 October 2004**

Ethereal

The Nobel Assembly at Karolinska Institutet has today decided to award

The Nobel Prize in Physiology or Medicine for 2004

jointly to

Richard Axel and Linda B. Buck

for their discoveries of

"odorant receptors and the organization of the olfactory system"

http://chemconnections.org/organic/chem226/Labs/Smell/ChemComm.html

#### Organic Chemistry

#### **Organic Functions & Smell Receptors.**

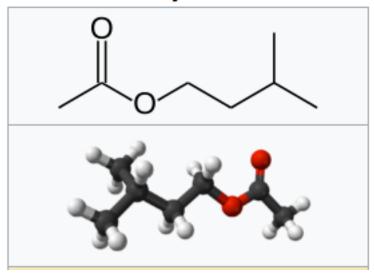
Table of organic compounds and their smells

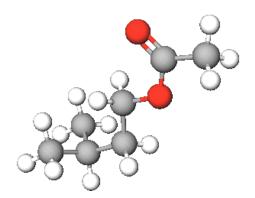
	ALK/	ANES	ALKENES	ALCO	HOLS		ALDE	HYDES		KETO	ONES	CARBOXY	LIC ACIDS		HALOALKANE	S	THIOLS	AMI	NES	NITRILES	LACTONI
	-ane	cyclo -ane	-ene	-anol	-an-2-ol	-anal	2-methyl -anal	3-(4-t-butylphenyl) -anal	-enal	-an-2-one	methyl -an-2-one	-anoic acid	-enoic acid	chloro -ane	bromo -ane	iodo -ane	-anethiol	-anamine	diamino -ane	-anenitrile	-anolide
on	none	doesn't exist	carbene is too unstable to smell	ABSOLUT	doesn't exist	FORMAL DEHYDE MINTANT & POTENTIAL CANCEL HAZARD AUTOMISS PRINCIPAL OUT	doesn't exist	doesn't exist	doesn't exist	doesn't exist	doesn't exist	PUNGENT & PENETRATING	doesn't exist	TOXIC & MILDLY SWEET	LIKE CHLOROFORM	SWEET, ACRID	<b>100</b>	7	?		doesn't ex
ons	none	doesn't exist		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 ex
ons	none	- D		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
ons	none	1	<b>6</b>		gonfuls WINE	PUNGENT	SP.	LILY	PUNGENT & SUFFOCATING	BUTTERSCOTCH	LIKE NAIL VARNISH REMOVER	RANCID BUTTER	BROWN	SHARP	PLEASANT, SWEET	SHARP, UNIQUE	butanethiol skunk 3-methyl butan-3-thiol ratural gas odorani		DEAD	SUFFOCATING	9
ons	STARTING FLUID	PLEASANT	<u>• 0</u>	STRONG SWEET	(S)- and (R)- enantiomers	PUNGENT NUTS & CHOCOLATE	FRESHLY CUT GRASS	?		8	MINT (4-methyl-)	DISGUSTING		MILD	PLEASANT, SWEET		ROASTED		DEAD ANIMALS & URINE		HERBA
.0115	STA <mark>RT</mark> ING FLUID	SWEET	<b>600</b>	FRESHLY CUT GRASS	7	FRESHLY CUT GRASS	FRESHLY CUT GRASS	?	J	ATTRACTS	(3-methyl-)	GOATS	ARMPITS (WHEN 3- METHYLATED)	AROMATIC	SLIGHTLY	?	BURNED		ROTTING FISH		€ & €
naming used	n/a	n/a	Benzene	SICKENINGLY SWEET AND TARRY Phenol	doesn't exist	800 P	***	?	doesn't exist	doesn't exist	Acetophenone	BALSAMIC	doesn't exist		AROMATIC	•	<b>W</b> •••	Aniline	TOXIC, AROMATIC	Benzonitrile	doesn't e
ons			<b>600</b>	FRESHLY CUT GRASS	(S)- and (R)- enantiomers	STRONG, FRUITY COGNAC	(2,6-dimethy) heptanal)	?	ALMOND BUTTER	4	(6-methyl-)	RANCID	ARMOTTS (WHEN 3- METHYLATED)	none	SLIGHTLY	none					CARAMEI &
oons	PETRO	•	1	PENETRATING, SWEET	(S)- and (R)- enantiomers	STRONG, CITRUS- LIKE	?	?	80	-2-one petrol -3-one herb butter	?	M <sub>a</sub>	ARMPITS	none		SEAWEED	STENCH	7			
oons	DIESEL		<del>O</del>	CITRUS	<b>S</b>	ATTRACTS MOSQUITOES		?	OLD PEOPLE	MILK	?	RANCID	ARMPITS	none	none	none	OBNOXIOUS			<u>^</u>	
-	JET FUEL	•	<del>O</del>	FLOWERS	?	BUCKWHEAT		?	TALLOW	?	?	M	ARMPITS	none	none	none	OBNOXIOUS				
bons	ALSO ANT PANIC PHEROMONE	?	<del>O</del>	FLOWERS	?	MAKES SPERM UNABLE TO FIND THE EGG	KUMQUATS	?		ALGERIAN OIL OF RUE	?	WAXY	PUNGENT & PENETRATING	UNIQUE & UNPLEASANT	none	MOUSE PHEROMONE	OBNOXIOUS			<u>^</u>	& (
bons	STINKSBUG	MUSTY	· A	FLOWERS	?		?	?	å ()	?	?	BAY OIL	FATTY	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS				<b>A</b>
DOIIS	PHEROMONE	FOUND IN ROSES	- D	PLEASANT	?	GRAPEFRUIT PEEL	ROASTED	?	?	WAXY	?		?	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS		none	<u>^</u>	ANGEL
	KAPOK BUSH FLOWERS	none	- D		?		?	?	?	?	?	WAX & NUTMEG	?	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS		none		CED/ WOO
bons	TAMARIND	?			?	FRESH	?	?	CORIANDER	CELERY	?	FOR DAIRY CONSUMPTION (No smell)	?	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS		none	$\triangle$	₩.

#### One molecule, one function: One Smell Receptor

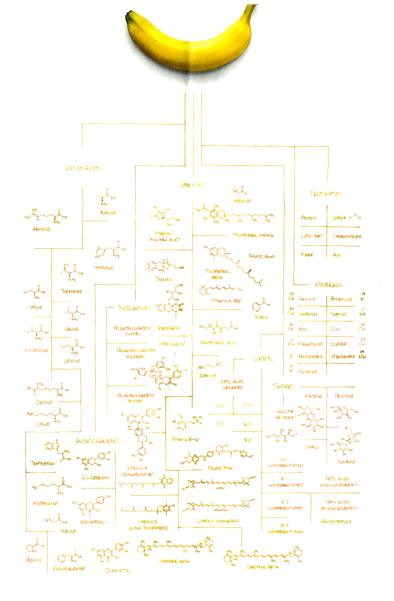
Isoamyl acetate, also known as isopentyl acetate, is formed from isoamyl alcohol and acetic acid. It is a colorless liquid that is only slightly soluble in water, but very soluble in most organic solvents. Isoamyl acetate has a strong odor which is also described as similar to both banana and pear.[3] Banana oil may be either pure isoamyl acetate, or flavorings that are mixtures of isoamyl acetate, amyl acetate, and other flavors.

#### Isoamyl acetate





 $C_7H_{14}O_2$ 

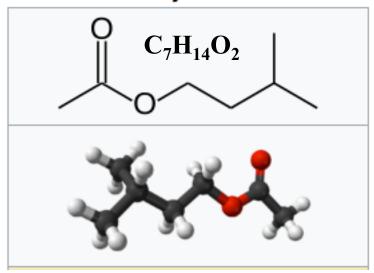


These are just some of the 82 primary chemicals that make up a natural, delicious banana. Everything is chemistry. Discover what's inside our products at whatsinsidescjohnson.com.

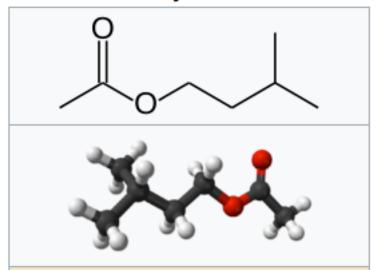


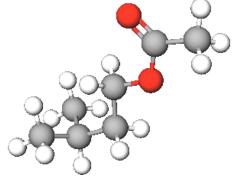
## One molecule among 82 primary chemicals found in bananas:

#### Isoamyl acetate



#### Isoamyl acetate





 $C_7H_{14}O_2$ 

The function in isoamyl acetate's structure is a(n):

A.Alcohol

B.Aldehyde

C.Ketone

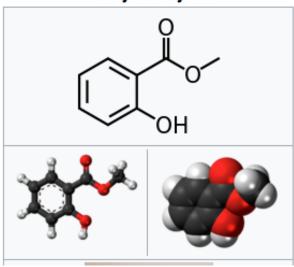
D.Ester

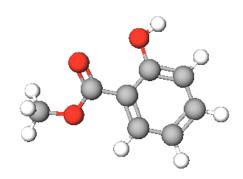
E.Carboxylic Acid

#### One molecule, two functions: One Smell Receptor

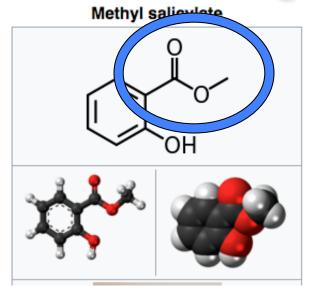
Methyl salicylate (oil of wintergreen or wintergreen oil) is naturally produced by many species of plants, particularly wintergreens. It is also synthetically produced, used as a fragrance, in foods and beverages, and in liniments.

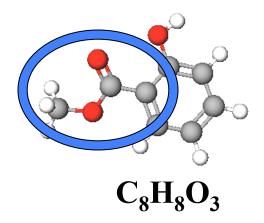
#### Methyl salicylate





 $C_8H_8O_3$ 





One of the functions, an ester, is circled. What is the other function?:

A.Alcohol

B.Ether

C.Ketone

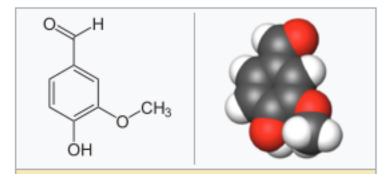
D.Aldehyde

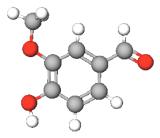
E.Carboxylic Acid

#### One molecule, three functions: One Smell Receptor

An extract of the cured, full-grown, unripe fruit of an orchid produces a popular flavoring. The natural extract sells for  $\sim $1500/kg$  versus  $\sim$  \$20/kg for the synthetic version. The structure of the compound that is responsible for the smell/flavor is shown to the right. The Guinness Book of World Records once listed this compound as having the lowest smell detection limit of all chemicals (2 x  $10^{-11}$  g per 1,000 cm<sup>3</sup> of air).

#### Vanillin

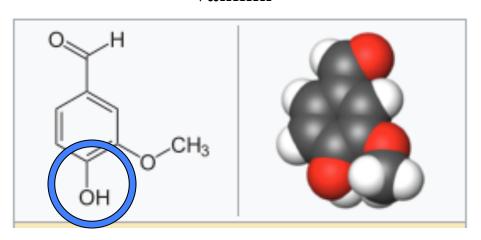


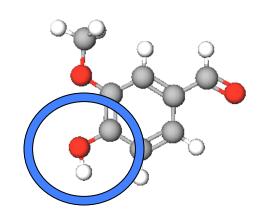


#### Bonus:

The space (volume) of the Oakland Coliseum Arena, aka Oracle Arena, is approximately  $90,000,000 \text{ ft}^3$ . If 1.00g of the compound were released at center court, and was completely and evenly dispersed throughout the building, would you smell it sitting in sec. 204, row H, seat 121? Show your calculation. (1  $\text{ft}^3 = 0.0283 \text{ m}^3$ )

#### Vanillin





One of the functions, an alcohol, is circled.

What are the other two functions?:

A.Aldehyde + Ketone

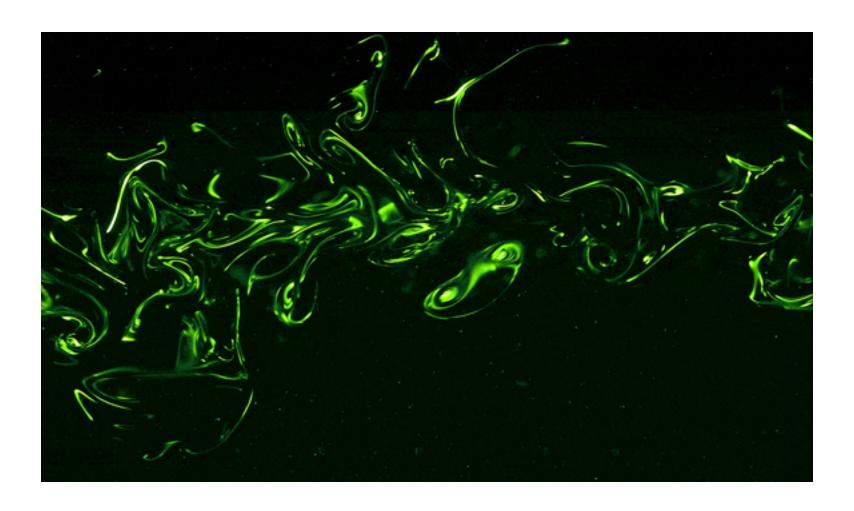
B.Carboxylic Acid + Ester

C.Ketone + Ether

D.Aldehyde + Ether

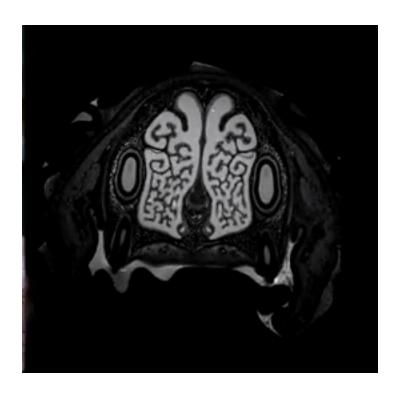
E.Carboxylic Acid + Aldehyde

#### What a smell looks like



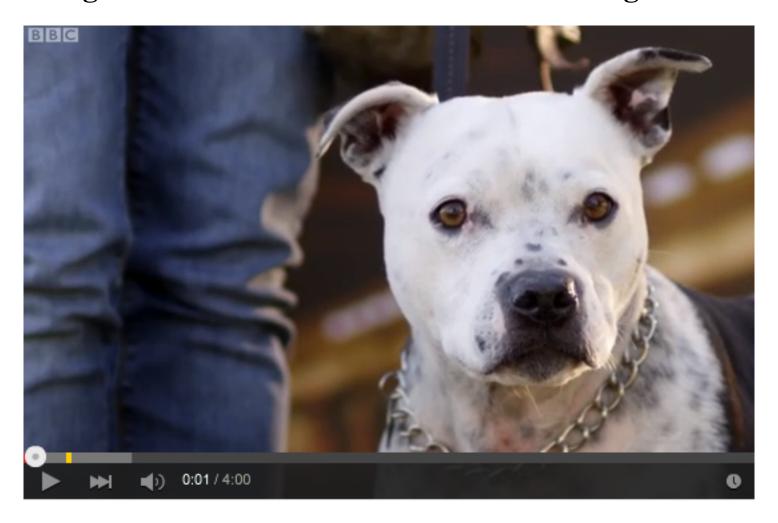
 $https://www.youtube.com/watch?v=58U52lDTuvk\&list=PLgawtcOBBjr9I-NDoUX-HmTQr\_VN465G2\&index=3$ 

#### Inside the extraordinary nose of a search-and-rescue dog



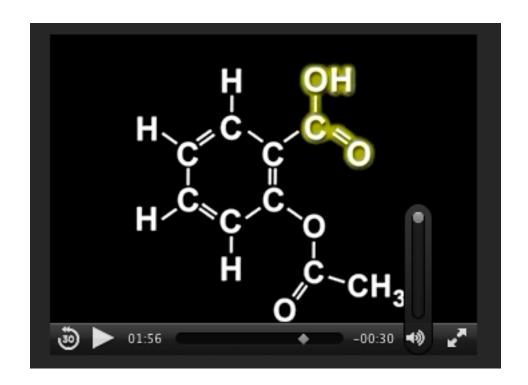
https://www.youtube.com/watch?v=FLH36ML8IEU

#### **Dogs Can Smell Cancer - Secret Life of Dogs - BBC**



https://www.youtube.com/watch?v=e0UK6kkS0\_M

## Synthesis of a Non-steroid anti-inflammatory drug Aspirin



http://chemconnections.org/general/movies/Representations.MOV

## Synthesis of a Nonsteroid antiinflammatory drug Aspirin & Pain



American Chemical Society



According to NIH, opioid-related drug overdoses lead to over 115 deaths each day in the United States alone. Unfortunately, for the almost one-third of Americans who suffer from chronic pain, prescription opioids continue to be their best choice for pain-relief.

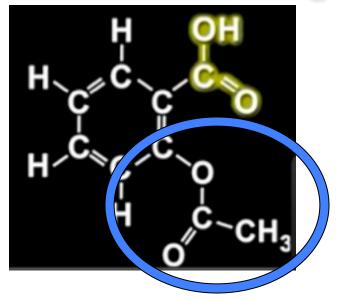


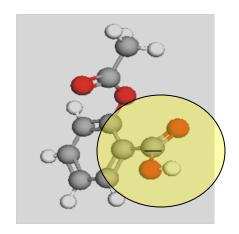
Join Ajay Yekkirala of Blue Therapeutics and Jane Aldrich of the University of Florida this **Thursday, May 10th from 2pm ET to 3pm ET** to discover how medicinal chemists are developing potent analgesics that are devoid of narcotic side effects to stop the cycle of pain-opioid abuse.

Register for Free!

#### What You Will Learn

- What are the stats, scientific issues, and policy ramifications driving the opioid crisis
- What are the body's pain pathways and where are the potential clinical targets
- The search for solutions and what are medicinal chemists working on right now





One of aspirin's functions, an ester, is circled in blue. What is the highlighted yellow function?:

A.Alcohol

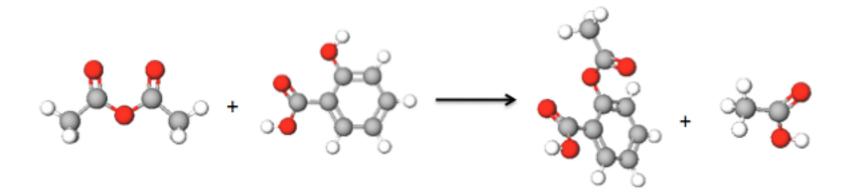
B.Ether

C.Ketone

D.Aldehyde

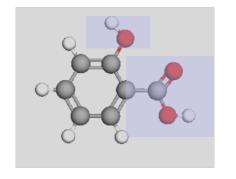
E.Carboxylic Acid

## Synthesis of Aspirin



## Salicylic Acid

#### Common Functional Groups



#### Name

#### **General Formula**

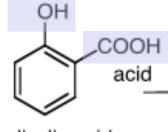
**Alcohols** 

R-OH

**Ethers** 

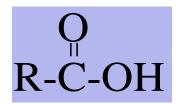
**Amines** 

alcohol (phenol)
OH



salicylic acid

**Carboxylic Acids** 



water	ammonia	methane	formaldehyde	formic acid
	3			

## **Aspirin**

#### Common Functional Groups

### **Name**

### **General Formula**

**Aldehydes** 

**Ketones** 

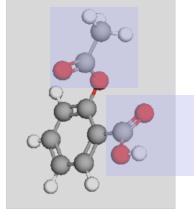
**Carboxylic Acids** 

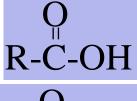
**Esters** 

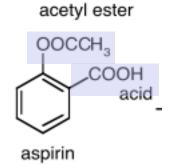
**Amides** 









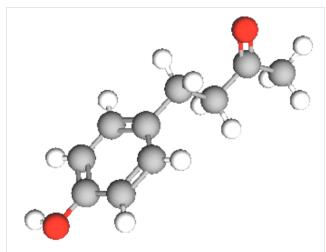


## Discussion Questions

http://chemconnections.org/general/chem108/Organic%20Chemistry%20Guide.html

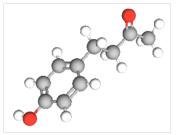
A compound that smells like fresh raspberries, the following structure, C<sub>?</sub>H<sub>?</sub>O<sub>?</sub>, matches its calculated molar mass which is 164 g/mol.

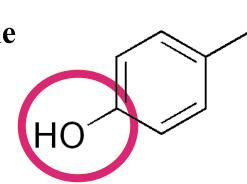
- A) TRUE
- B) FALSE





Select the function(s) in the molecule

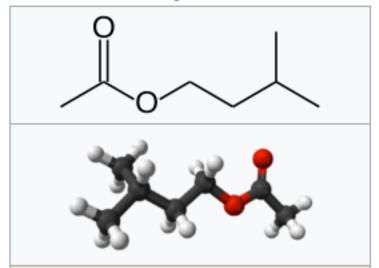


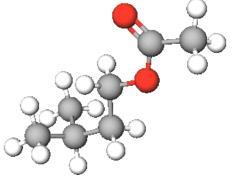


Alcohol	R-OH
Ether	R-O-R'
Amine	R-NH <sub>2</sub>
Aldehyde	O R-C-H
Ketone	R-C-R'
Carboxylic Acid	O R-C-OH
Ester	R- $C$ - $OR'$ $Q$ $R''$
Amide	R-C-N



#### Isoamyl acetate





 $C_7H_{14}O_2$ 

The function in isoamyl acetate's structure is a(n):

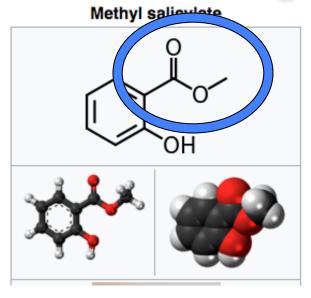
A.Alcohol

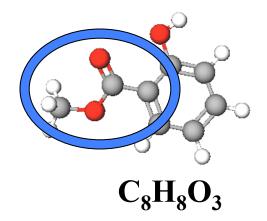
B.Aldehyde

C.Ketone

D.Ester

E.Carboxylic Acid





One of the functions, an ester, is circled. What is the other function?:

A.Alcohol

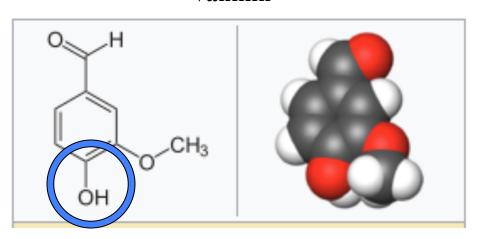
B.Ether

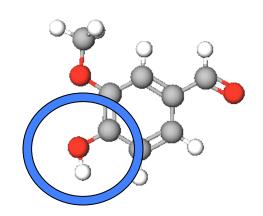
C.Ketone

D.Aldehyde

E.Carboxylic Acid

#### Vanillin





One of the functions, an alcohol, is circled.

What are the other two functions?:

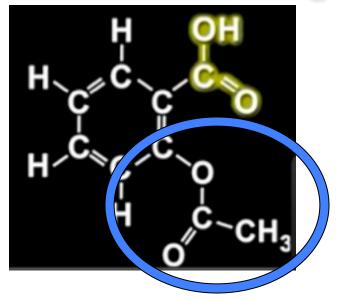
A.Aldehyde + Ketone

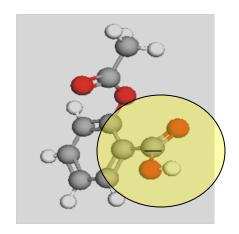
B.Carboxylic Acid + Ester

C.Ketone + Ether

D.Aldehyde + Ether

E.Carboxylic Acid + Aldehyde





One of aspirin's functions, an ester, is circled in blue. What is the highlighted yellow function?:

A.Alcohol

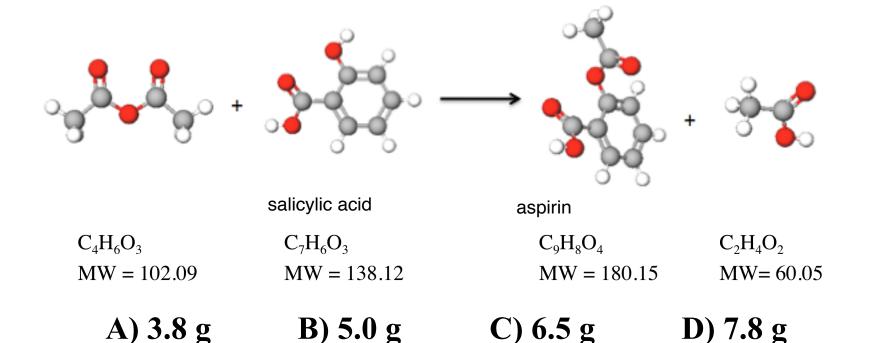
B.Ether

C.Ketone

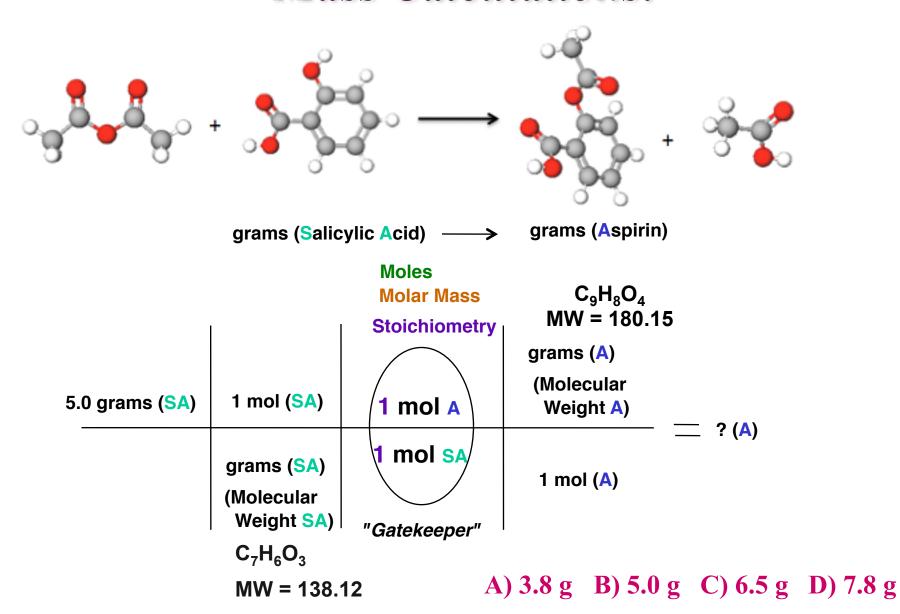
D.Aldehyde

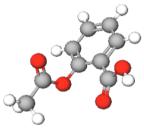
E.Carboxylic Acid

- How many grams of aspirin can be theoretically produced from 5.0 g of salicylic acid reacting with an excess of acetic anhydride,  $C_4H_6O_3$ ?
- Balanced Equation:



#### Mass Calculations:





A Kaitlyn's synthesis of aspirin, C<sub>9</sub>H<sub>8</sub>O<sub>2</sub>, produced 5.90g. The calculated theoretical yield was 6.50g; what is her % yield?

A) 47.5% B) 80.3% C) 90.6%

D) 110%

