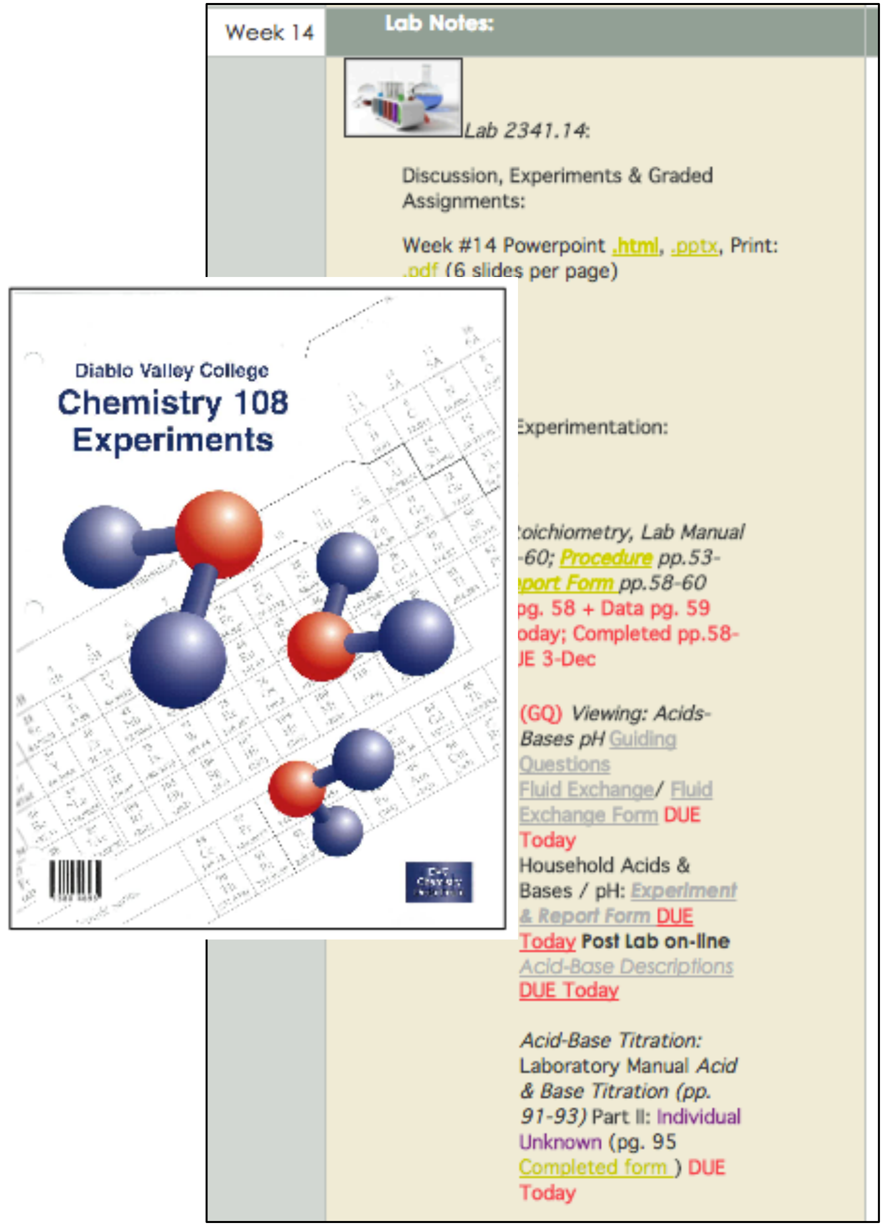
Chem 108: Lab

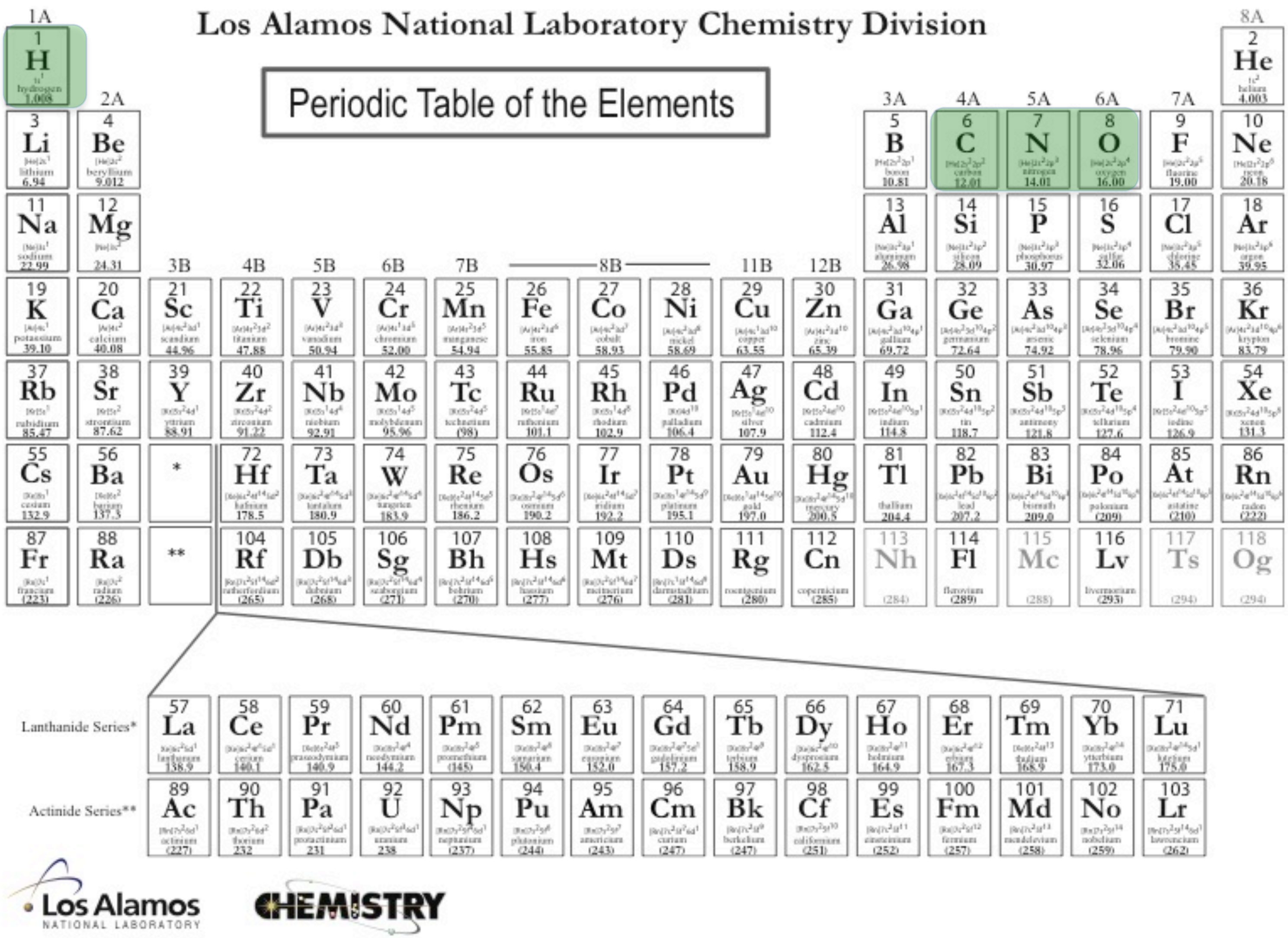
Week 16

Sign in
Pick up papers
& handout

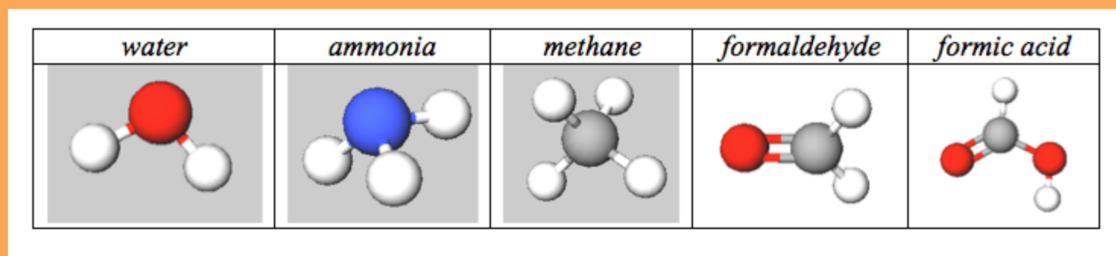
Experiment:
Synthesis of Aspirin
pp.87-91



Elemental building blocks for all organic molecules



Organic Molecules



Shapes, Functions & Structural Analogies

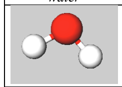
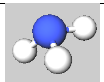
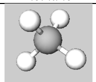
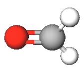
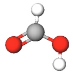
Water, Ammonia, Methane

Plus >C=O “carbonyls”

Functional Groups & Amino Acids

Organic Molecules & Functional Groups

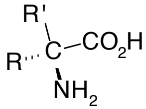
The following simple molecules: water, ammonia, methane, formaldehyde and formic acid can be used as "lego-like" building blocks to construct the vast majority of organic and biological molecules. Simply replace a hydrogen from each of any two molecules with a bond to the central atom, and if joining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

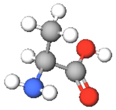
water	*ammonia*	*methane*	*formaldehyde*	*formic acid*
				

Name	**General Formula**
Alcohols	R–OH
Ethers	R–O–R′
Amines	$R–NH_2$
Carboxylic Acids	R-C(=O)-OH

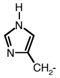
Aldehydes	R-C(=O)-H
Ketones	R-C(=O)-R'
Carboxylic Acids	R-C(=O)-OH
Esters	R-C(=O)-OR'
Amides	R-C(=O)-N(R")R'

20 Amino Acids found in Proteins of Living Organisms





https://chem.libretexts.org/LibreTexts/Diablo_Valley_College/DVC_Chem_106%3A_Rusay/Amino_Acids

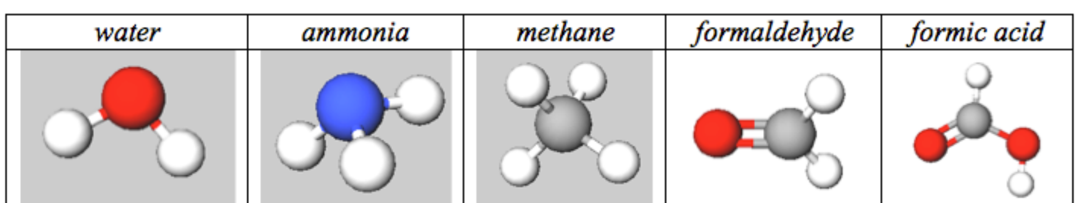
Name	I	II	R-	R'-	Rasmol Color	Function & Class
Alanine	Ala	A	H-	CH_3-	dark gray	Aliphatic Hydrophobic
Arginine	Arg	R	H-	$-CH_2CH_2CH_2NHC(=NH)NH_2$	blue	Basic Hydrophilic
Asparagine	Asn	N	H-	$-CH_2C(=O)NH_2$	cyan	Amide Highly Hydrophilic
Aspartate	Asp	D	H-	$-CH_2C(=O)OH$	bright red	Acidic Hydrophilic
Cysteine	Cys	C	H-	$-CH_2SH$	yellow	Sulphur Containing Hydrophobic
Glutamine	Gln	Q	H-	$-CH_2CH_2C(=O)NH_2$	cyan	Amide Highly Hydrophilic
Glutamate	Glu	E	H-	$-CH_2CH_2C(=O)OH$	bright red	Acidic Hydrophilic
Glycine	Gly	G	H-	H-	light gray	Aliphatic Hydrophobic
Histidine	His	H	H-		pale blue	Basic Hydrophilic
Isoleucine	Ile	I	H-	$-CH(CH_3)CH_2CH_3$	green	Aliphatic Hydrophobic
Leucine	Leu	L	H-	$-CH_2CH(CH_3)CH_3$	green	Aliphatic Hydrophobic

Organic Molecules

Common Functional Groups

Name	General Formula
Alcohols	R−OH
Ethers	R−O−R′
Amines	R−NH_2
Carboxylic Acids	O ‖ R-C-OH

R′− or R− represents any generic carbon atom bonded in the functional group

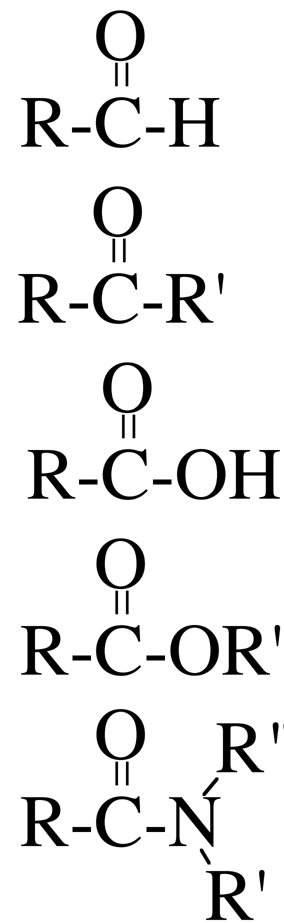


Organic Molecules

Common Functional Groups

Name	General Formula
Aldehydes	
Ketones	
Carboxylic Acids	
Esters	
Amides	

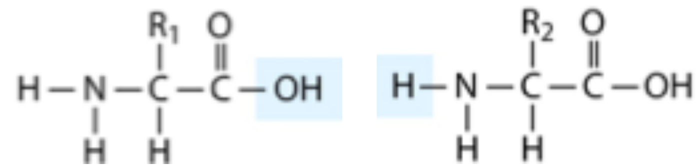
R′– or R– represents any generic carbon atom bonded in the functional group

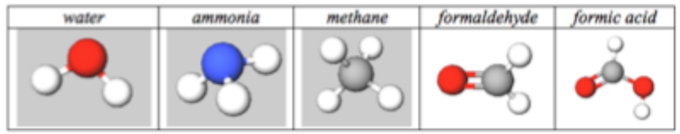


Amino acids: two functions, an acid & a base, in the same molecule

Amines $R-NH_2$

Carboxylic Acids $R-C(=O)-OH$

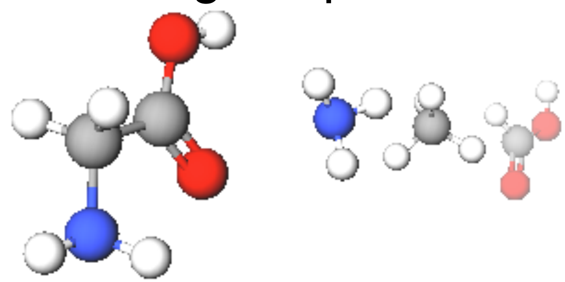




	Functions	
	Alcohol	$R-OH$
	Ether	$R-O-R'$
X	Amine	$R-NH_2$
	Aldehyde	$R-C(=O)-H$
	Ketone	$R-C(=O)-R'$
X	Carboxylic Acid	$R-C(=O)-OH$
	Ester	$R-C(=O)-OR'$
	Amide	$R-C(=O)-NR'R''$

Amino Acids
Legos of Chemical Biology

Amino acids containing carbon, hydrogen, oxygen, and nitrogen, which resemble the following shapes & structural components



•20 different amino acids are encoded in humans' genetic code, which is archived in DNA.

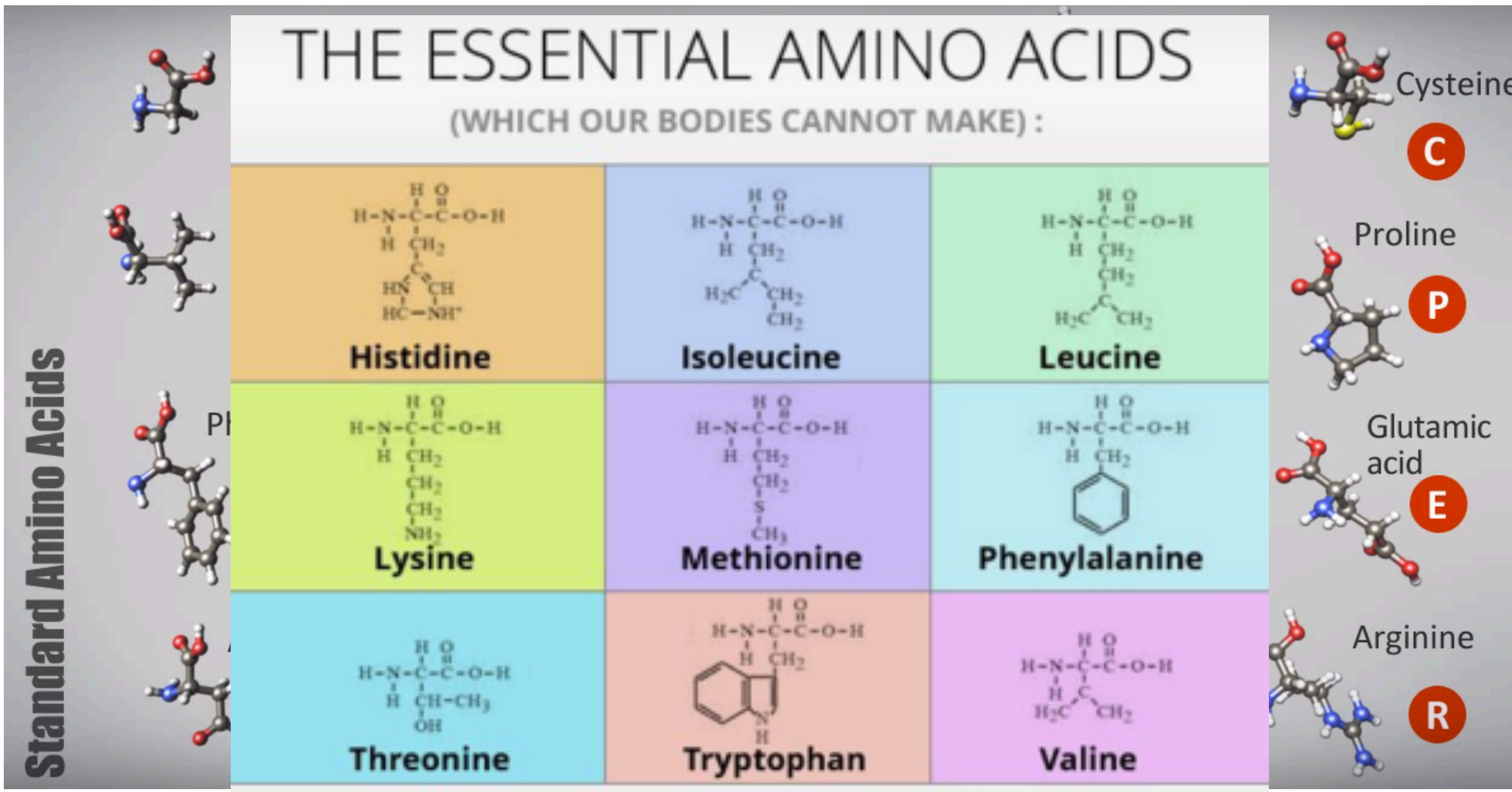
•Hundreds of amino acids link together with amide (peptide) bonds to form proteins, which provide the machinery and molecular backbone for the chemistry of life.

•There are less than 20,000 total proteins produced from humans' entire genome, each coded by a specific gene in DNA's ~3 billion genetic bases.

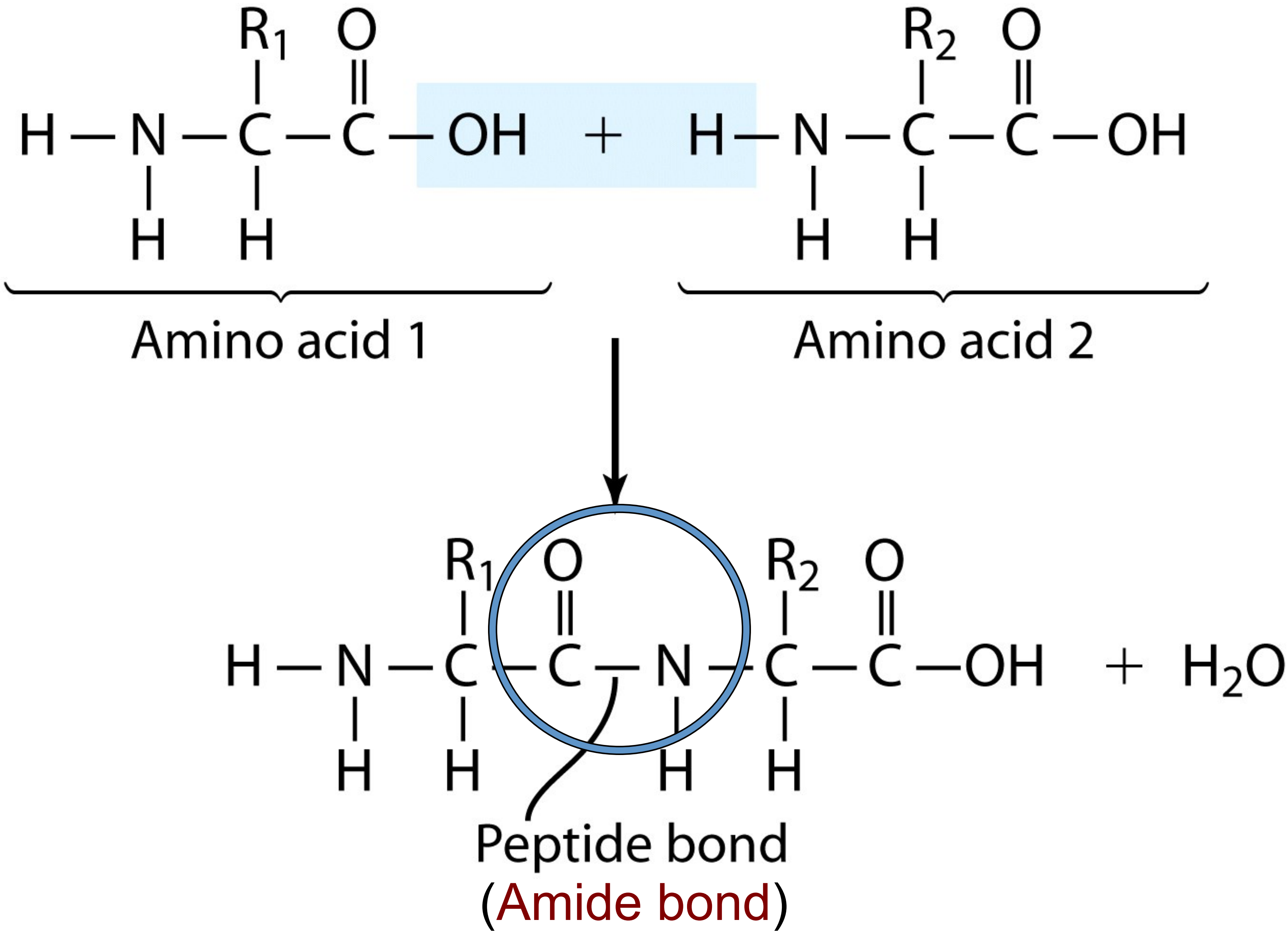
http://chem.libretexts.org/LibreTexts/Diablo_Valley_College/DVC_Chem_106%3A_Rusay/Amino_Acids

Amino Acids
Legos of Chemical Biology

All amino acids contain C, H, O, and N; two, C & M. also have sulfur.



http://chem.libretexts.org/LibreTexts/Diablo_Valley_College/DVC_Chem_106%3A_Rusay/Amino_Acids

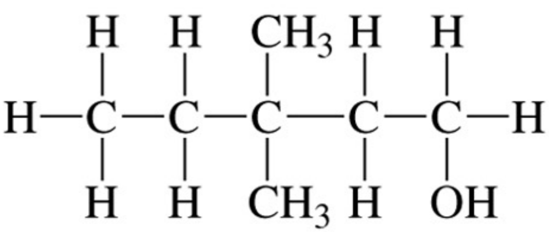

R1 O
H — N — C — C — OH + H — N — C — C — OH
H H H H
R2 O
Amino acid 1
Amino acid 2
R1 O R2 O
H — N — C — C — N — C — C — OH + H2O
H H H H
Peptide bond
(Amide bond)

Representing Organic Molecules

Common Formulas & Drawings

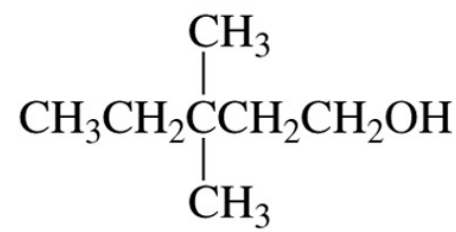
Molecular formula: $C_7H_{16}O$

Empirical Formula: $C_7H_{16}O$

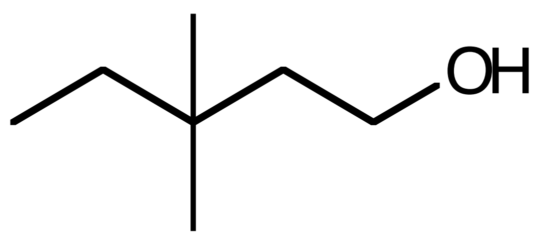


Condensed Structure:

$CH_3CH_2C(CH_3)_2CH_2CH_2OH$ or



Bond-Line Structure:



Organic Molecular Jeopardy

Team Selection

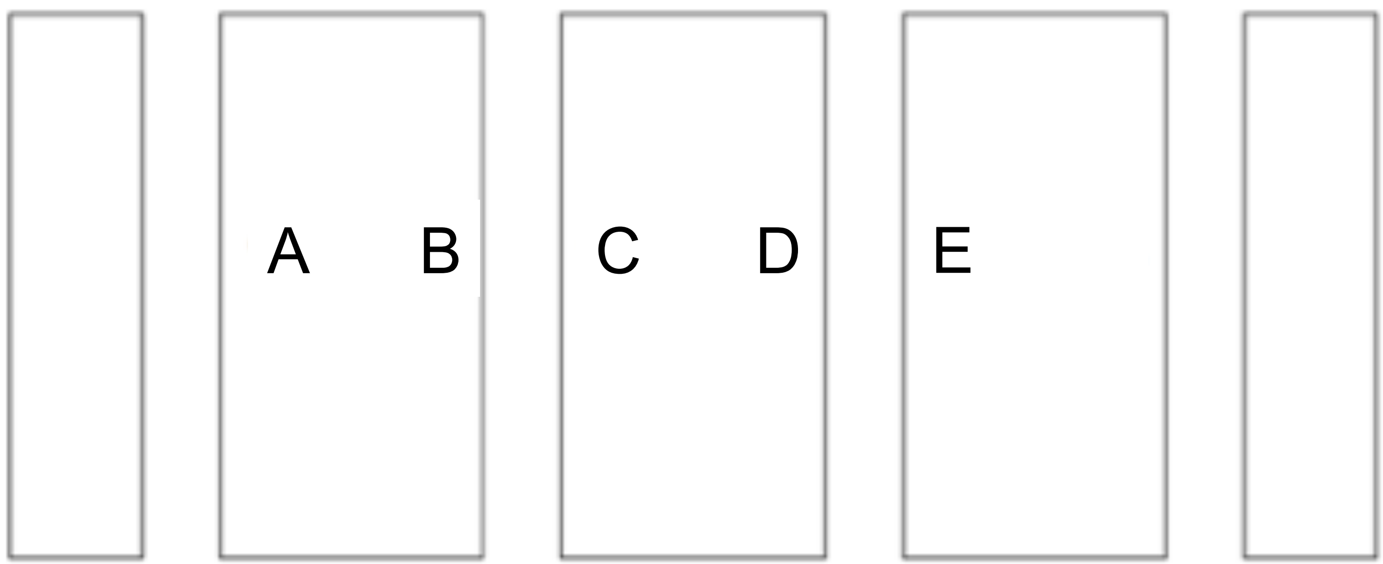
Organic Molecular Jeopardy

Team Selection

Pick a card & write your name on the card.

Go to the lab location noted on the map.

Front of Lab



Organic Molecular Jeopardy

Team Reporting

Select a Team Scribe:

Record the full names of your Team on the form Dr. R. provides and return it to him when complete.

Organic Molecular Jeopardy	
TEAM:	
	Members
1	
2	
3	
4	
5	

Organic Molecular Jeopardy

SCORING

There will be 7 questions (5pts each) embedded in the lab presentation; plus a final jeopardy question (15pts).

Dr. R will explain the rules. Lab bonus points will be awarded.

1st place: 25 pts

2nd place: 15 pts

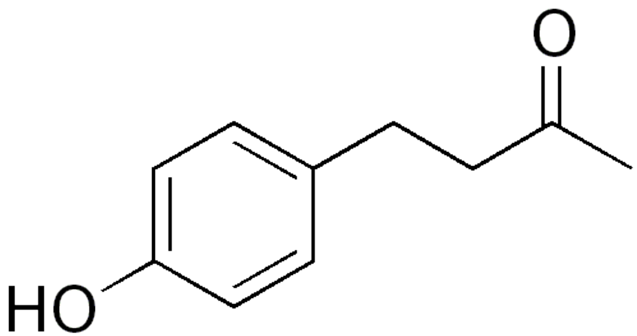
3rd place: 10 pts

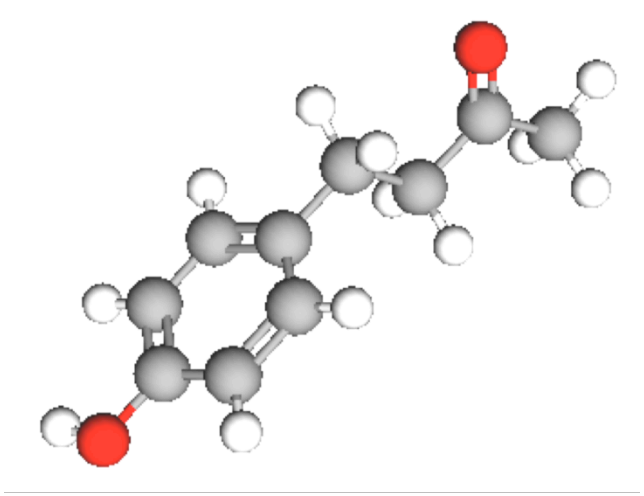
Other participant scoring: 5 pts

Organic Molecular Jeopardy

Common Formulas & Drawings

A compound that smells like fresh raspberries, is shown below. What is its molecular formula and molar mass?

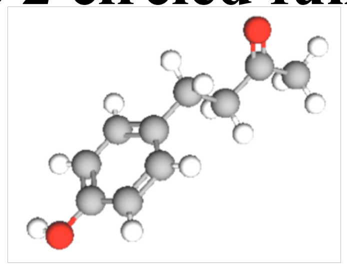


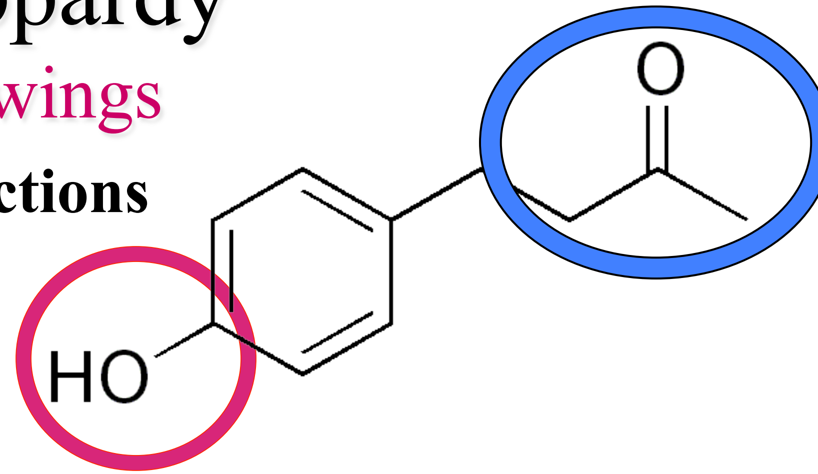


Organic Molecular Jeopardy

Common Formulas & Drawings

Select the names of the 2 circled functions in the molecule.

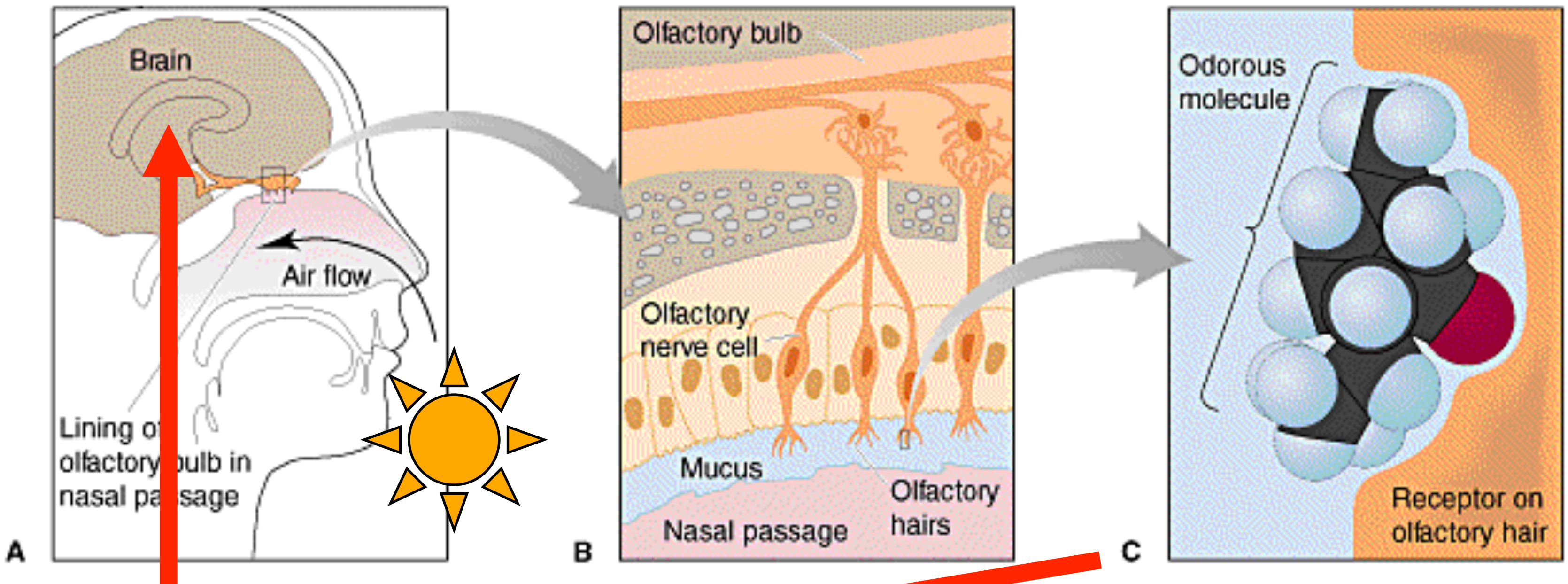




	Alcohol	R−OH
	Ether	R−O−R′
	Amine	R−NH_2
	Aldehyde	R-C(=O)-H
	Ketone	R-C(=O)-R'
	Carboxylic Acid	R-C(=O)-OH
	Ester	R-C(=O)-OR'
	Amide	R-C(=O)-N(R')R"

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

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

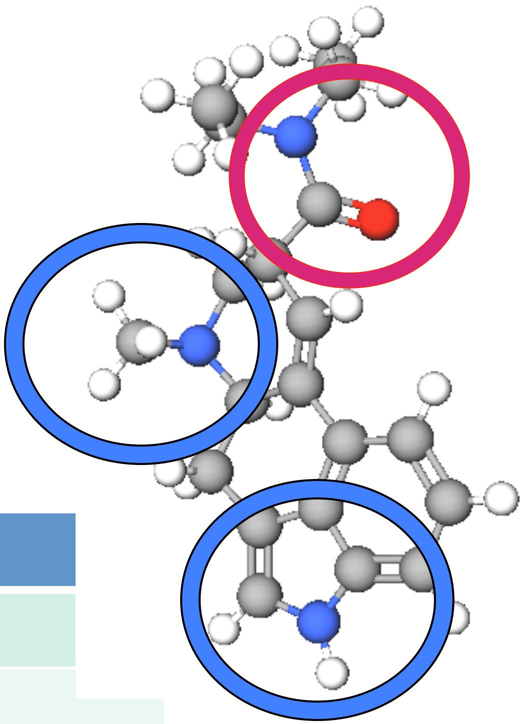


Structure-Odor Relationships
Karen J. Rossiter, Chem. Rev., 1996, 96, 3201-3240

Organic Molecular Jeopardy

Common Formulas & Drawings

This molecule may interfere with the perception of the smell of raspberry. What two functions are in the structure?



Alcohol	R−OH
Ether	R−O−R′
Amine	$R-NH_2$, R_2-NH, R_3-N
Aldehyde	R-C(=O)-H
Ketone	R-C(=O)-R'
Carboxylic Acid	R-C(=O)-OH
Ester	R-C(=O)-OR'
Amide	R-C(=O)-N(R')R"

Organic Functions & Smell Receptors.

Organic Chemistry
Table of organic compounds and their smells

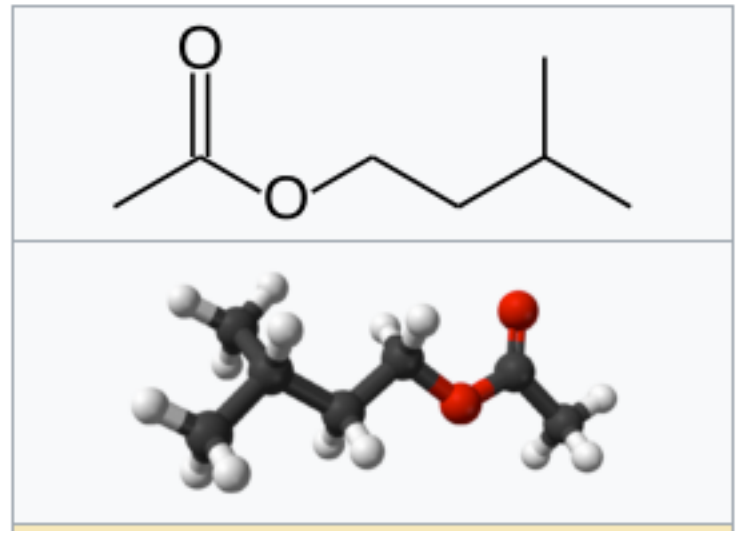
	ALKANES		ALKENES	ALCOHOLS		ALDEHYDES				KETONES		CARBOXYLIC ACIDS		HALOALKANES			THIOLS	AMINES		NITRILES	LACTONES
	-ane	cyclo -ane	-ene	-anol	-an-2-ol	-anal	2-methyl -anal	3-(4-t-butylphenyl) -anal	-enal	-an-2-one	methyl -an-2-one	-anoic acid	-enoic acid	chloro -ane	bromo -ane	iodo -ane	-anethiol	-anamine	diamino -ane	-anenitrile	-anolide
meth- 1 carbon	none	doesn't exist	carbene is too unstable to smell	ABSOLUT VODKA	doesn't exist	DANGER FORMALDEHYDE IRRITANT & POTENTIAL CANCER HAZARD AUTHORIZED PERSONNEL ONLY	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			?		doesn't exist
eth- 2 carbons	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	SWEET, ACRID	ETHEREAL	SKUNK			ETHEREAL	doesn't exist
prop- 3 carbons	none			ABSOLUT VODKA	RUBBING ALCOHOL	IRRITATING GREEN COFFEE	WET CEREAL	ATTRACTS SPERM	BURNED GREASE	NAIL VARNISH REMOVER	doesn't exist	SLIGHTLY RANCID	SHARP	MILDLY SWEET	SWEET	SHARP, UNIQUE				ETHEREAL	none
but- 4 carbons	none				WINE	PUNGENT BANANA		LILY	PUNGENT & SUFFOCATING	BUTTERSCOTCH	LIKE NAIL VARNISH REMOVER	RANCID BUTTER	BROWN SUGAR	SHARP	PLEASANT, SWEET	SHARP, UNIQUE	butanethiol skunk 2-methyl butan-2-thiol natural gas odorant		DEAD ANIMALS	SUFFOCATING	
pent- 5 carbons	STARTING FLUID	PLEASANT		STRONG SWEET	(S)- and (R)- enantiomers	PUNGENT NUTS & CHOCOLATE	FRESHLY CUT GRASS	?		&	MINT (4-methyl-)	DISGUSTING		MILD	PLEASANT, SWEET		ROASTED GARLIC		DEAD ANIMALS & URINE		HERBAL
hex- 6 carbons	STARTING FLUID	SWEET		FRESHLY CUT GRASS		FRESHLY CUT GRASS	FRESHLY CUT GRASS	?		ATTRACTS MICE	(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			?	doesn't exist	doesn't exist	Acetophenone	BALSAMIC	doesn't exist		AROMATIC			Aniline	TOXIC, AROMATIC	Benzonitrile	doesn't exist
hept- 7 carbons				FRESHLY CUT GRASS	(S)- and (R)- enantiomers	STRONG, FRUITY COGNAC	(2,6-dimethyl-heptanal)	?	ALMOND BUTTER	&	BAD (6-methyl-)	RANCID	ARMPITS (WHEN 3-METHYLATED)	none	SLIGHTLY SWEET	none	&				CARAMEL &
oct- 8 carbons	PETROL			PENETRATING, SWEET	(S)- and (R)- enantiomers	STRONG, CITRUS-LIKE	?	?		-2-one petrol -3-one herb butter	?	&	ARMPITS	none		SEAWEED	STENCH				
non- 9 carbons	DIESEL			CITRUS		ATTRACTS MOSQUITOES		?	OLD PEOPLE	MILK	?	RANCID	ARMPITS	none	none	none	OBNOXIOUS				
dec- 10 carbons	JET FUEL			CITRUS FLOWERS	?	BUCKWHEAT		?	ATORA TALLOW	?	?		ARMPITS	none	none	none	OBNOXIOUS				
undec- 11 carbons	NEW JET FUEL ALSO ANT 'PANIC' PHEROMONE	?		CITRUS FLOWERS	?	MAKES SPERM UNABLE TO FIND THE EGG	KUMQUATS	?	&	ALGERIAN OIL OF RUE	?	WAXY	PUNGENT & PENETRATING	UNIQUE & UNPLEASANT	none	MOUSE PHEROMONE	OBNOXIOUS				&
dodec- 12 carbons		MUSTY		FLOWERS	?		?	?	&	?	?	BAY OIL	FATTY	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS				&
tridec- 13 carbons	STINK-BUG PHEROMONE	UNIQUE; FOUND IN ROSES		PLEASANT	?	GRAPEFRUIT PEEL	ROASTED	?	?	WAXY	?		?	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS		none		ANGELICA ROOT
tetradec- 14 carbons	KAPOK BUSH FLOWERS	none			?		?	?	?	?	?	WAX & NUTMEG	?	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS		none		CEDAR WOOD
pentadec- 15 carbons	TAMARIND (ANT-CALMING PHEROMONE)	?		ABSOLUT VODKA	?	FRESH	?	?	CORIANDER	CELERY	?	BIOMARKER FOR DAIRY CONSUMPTION (No smell)	?	UNIQUE & UNPLEASANT	none	?	OBNOXIOUS		none		MUSK

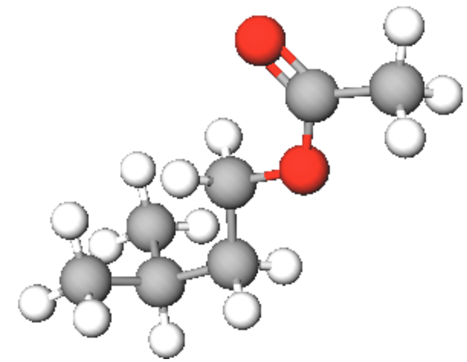
Version 1.2 Produced by James at jameskennedymonash.wordpress.com. Visit website for more infographics. Free to use!

One molecule, One function: One Smell Receptor

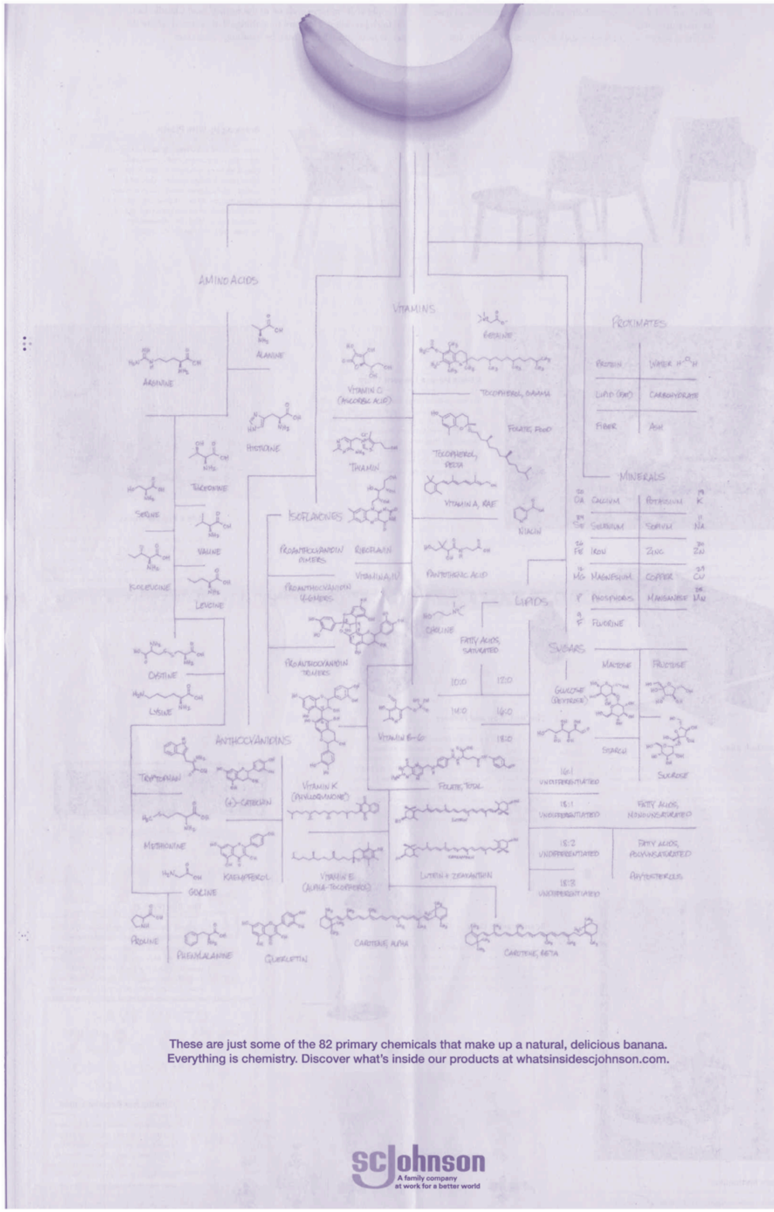
Isoamyl acetate, also known as isopentyl acetate, is formed from isoamyl alcohol and acetic acid. It is a colorless liquid that is only slightly soluble in water, but very soluble in most organic solvents. Isoamyl acetate has a strong odor which is also described as similar to both banana and pear. [3]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

Isoamyl acetate



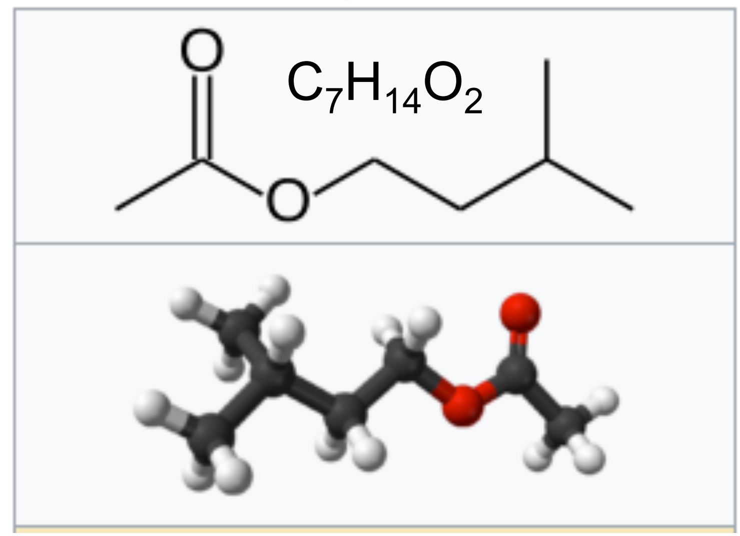


$C_7H_{14}O_2$



One molecule among 82 primary chemicals found in bananas:

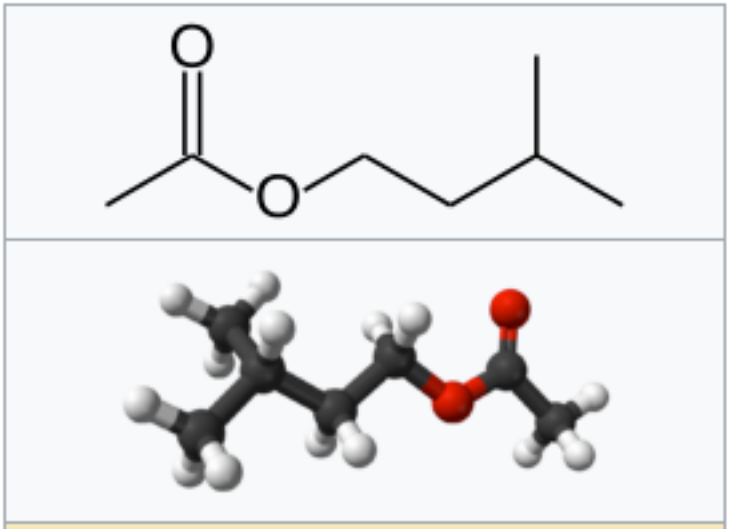
Isoamyl acetate

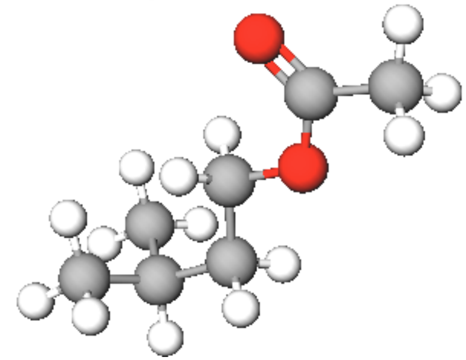


Organic Molecular Jeopardy

Common Formulas & Drawings

Isoamyl acetate





$C_7H_{14}O_2$

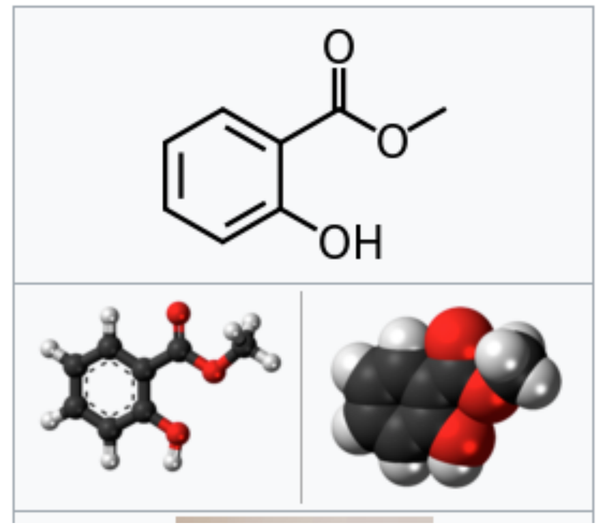
The function in isoamyl acetate's structure is a(n):

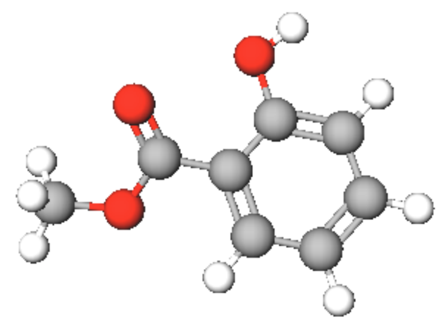
A. Alcohol
B. Aldehyde
C. Ketone
D. Ester
E. Carboxylic Acid

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

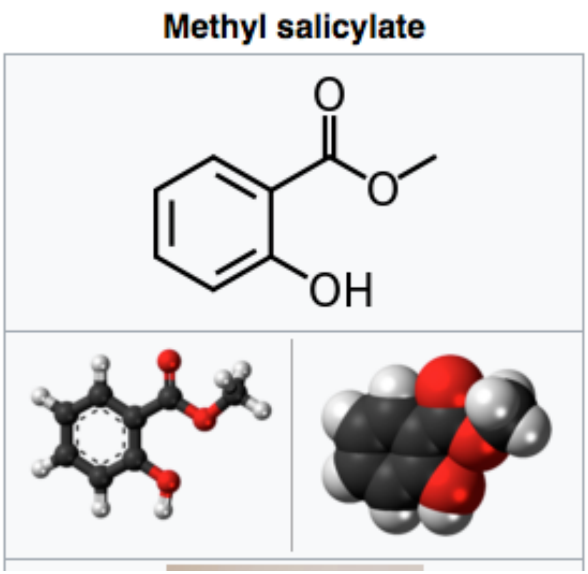


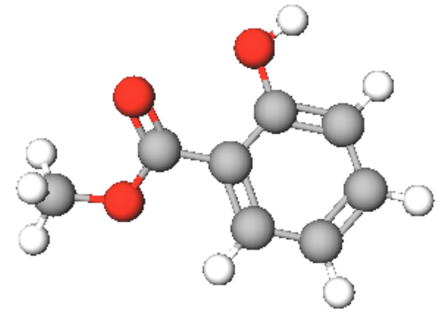


$C_8H_8O_3$

Organic Molecular Jeopardy

Common Formulas & Drawings





$C_8H_8O_3$

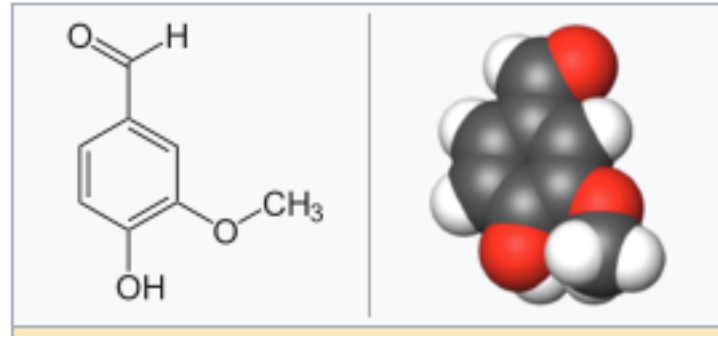
What are the 2 functions in methyl salicylate?

A. Alcohol
B. Ether
C. Ketone
D. Aldehyde
E. Carboxylic Acid
F. Ester

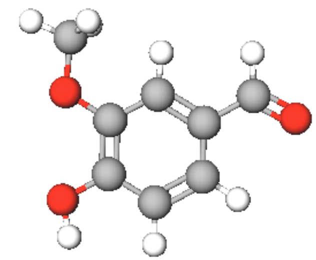
One molecule, three functions: One Smell Receptor

An extract of the cured, full-grown, unripe fruit of an orchid produces a popular flavoring. The natural extract sells for ~ $1500/kg versus ~ $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^3 of air).

Vanillin



$C_8H_8O_3$

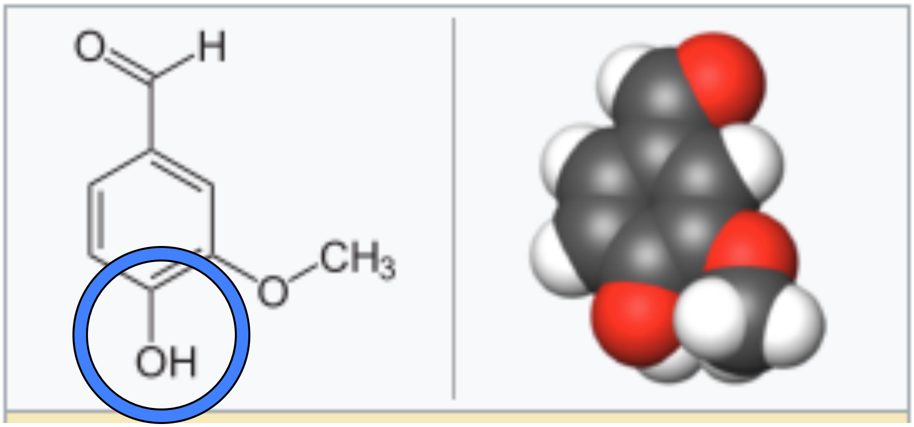


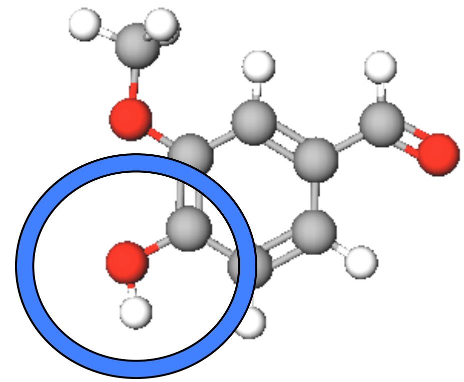
Bonus:
The space (volume) of the Oakland Coliseum Arena, aka Oracle Arena, is approximately 90,000,000 ft^3. If 1.00g of the compound were released at center court, and was completely and evenly dispersed throughout the building, would you smell it sitting in sec. 204, row H, seat 121? Show your calculation.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

Organic Molecular Jeopardy

Common Formulas & Drawings

Vanillin





$C_8H_8O_3$

One function, an alcohol, is circled. What are the other two functions?:

A. Aldehyde + Ketone

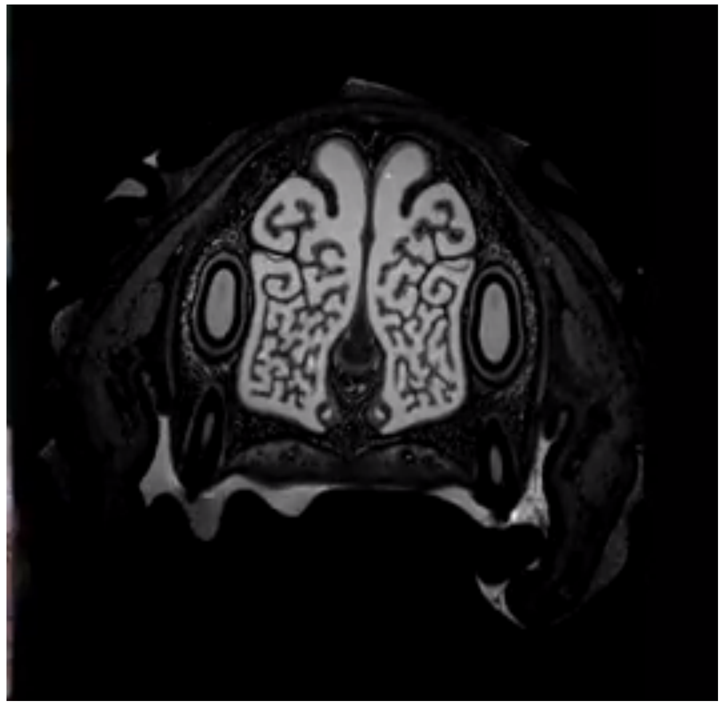
B. Carboxylic Acid + Ester

C. Ketone + Ether

D. Aldehyde + Ether

E. Carboxylic Acid + Aldehyde

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

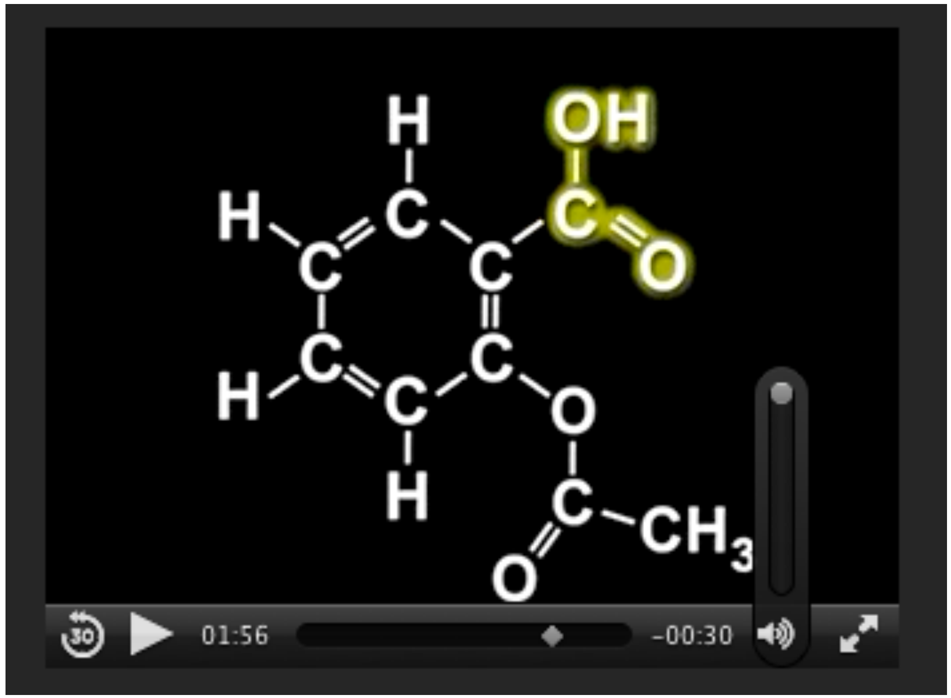


https://www.youtube.com/watch?v=FLH36ML8IEU

Dogs Can Smell Cancer - Secret Life of Dogs - BBC

https://www.youtube.com/watch?v=e0UK6kkS0_M

Synthesis of an NSAID
(Non-steroid anti-inflammatory drug)
Aspirin



$C_9H_8O_4$

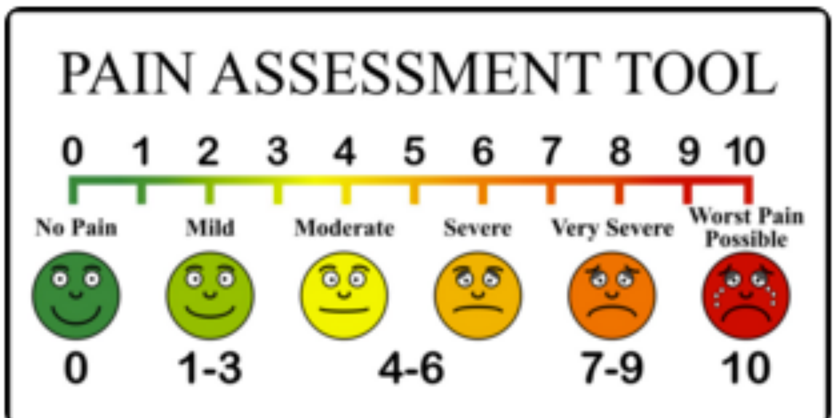
http://chemconnections.org/general/movies/Representations.MOV

NSAIDs are used primarily to treat inflammation, mild to moderate pain, and fever.

Synthesis of Aspirin (an NSAID)

Used primarily to treat inflammation, mild to moderate pain, and fever.

Aspirin & Pain



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.

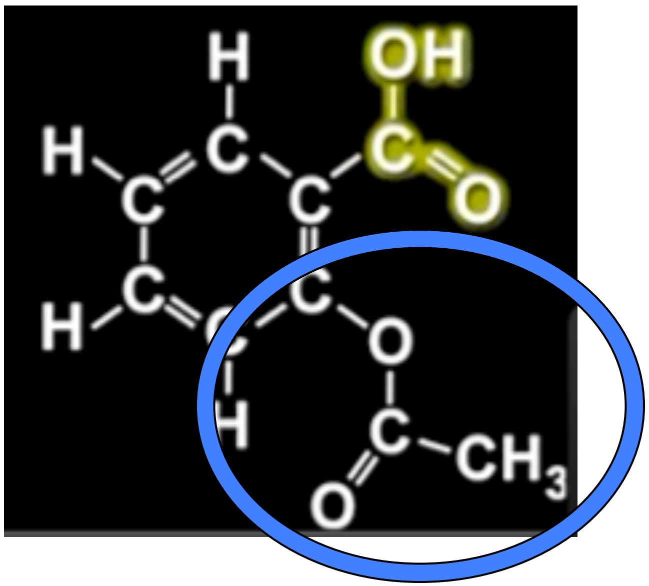
Register for Free!

What You Will Learn

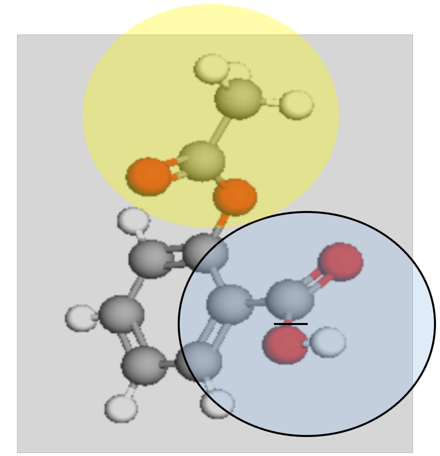
- What are the stats, scientific issues, and policy ramifications driving the opioid crisis
- What are the body's pain pathways and where are the potential clinical targets
- The search for solutions and what are medicinal chemists working on right now

Organic Molecular Jeopardy

Common Formulas & Drawings



$C_9H_8O_4$



One of aspirin's two functions is highlighted in yellow, the other is circled. What are the two functions?

A. Highlight=Alcohol; Circled=Ester

B. Highlight=Aldehyde; Circled=Ether

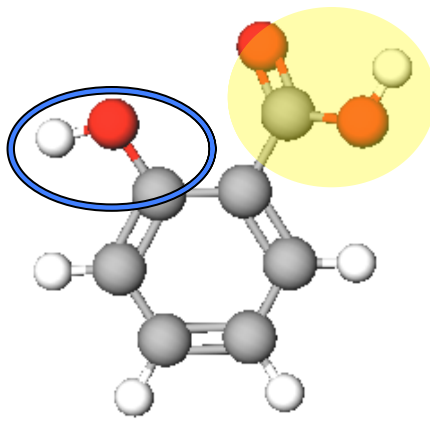
C. Highlight=Ketone; Circled=Alcohol

D. Highlight=Aldehyde; Circled=Ether

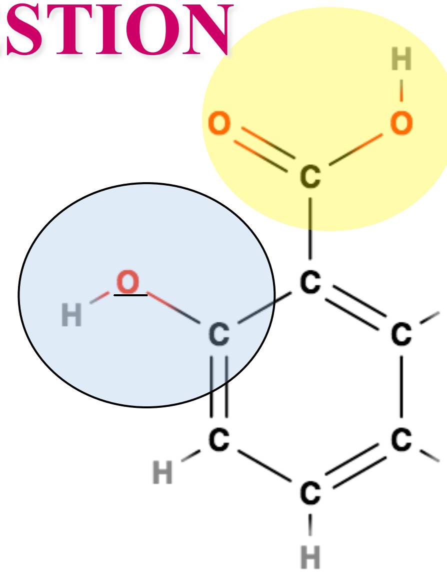
E. Highlight=Carboxylic Acid; Circled=Ester

Organic Molecular Jeopardy

FINAL JEOPARDY QUESTION



$C_7H_6O_3$



One of the reactants used to produce aspirin is shown above. It also has two functions: one is highlighted in yellow, the other is circled. What are the two functions?

A. Highlight=Alcohol; Circled=Ester

B. Highlight=Carboxylic Acid; Circled=Alcohol

C. Highlight=Ketone; Circled=Alcohol

D. Highlight=Aldehyde; Circled=Ether

E. Highlight=Carboxylic Acid; Circled=Ester

Organic Molecular Jeopardy

Tabulation

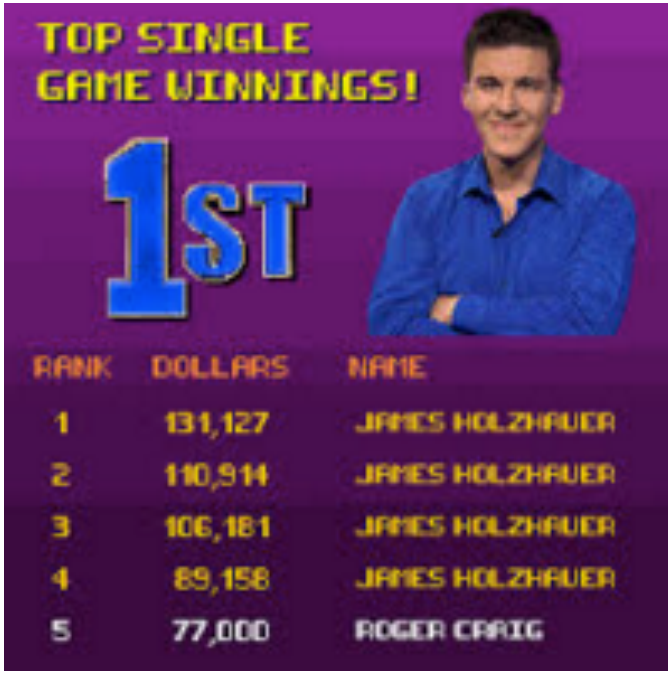
Organic Molecular Jeopardy					
	TEAMS:				
QUESTION	A	B	C	D	E
1					
2					
3					
4					
5					
6					
7					
FINAL					
TOTAL					

A word from our sponsor:

https://www.youtube.com/watch?v=hfe5xQ1M7Jw

Jeopardy

Winners



May 3, 2019

James Holzhauer, 22 days, $1,691,008

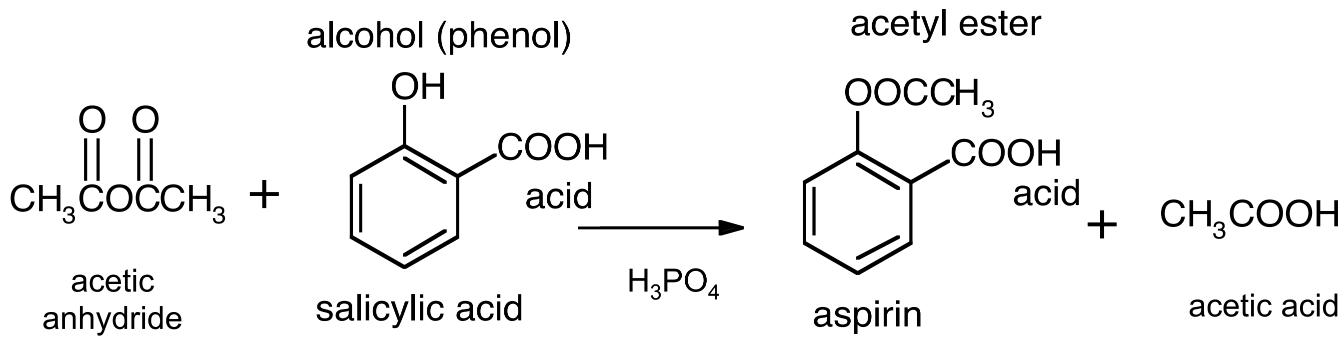
Organic Molecular Jeopardy

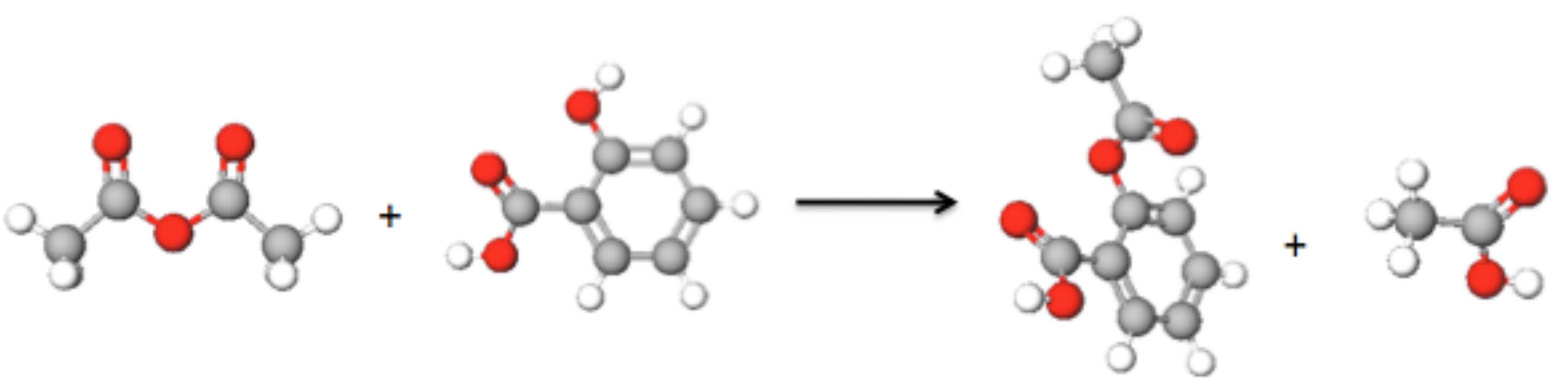
Winners

Organic Molecular Jeopardy					
	TEAMS:				
QUESTION	A	B	C	D	E
1					
2					
3					
4					
5					
6					
7					
FINAL					
TOTAL					

Select Partner(s): form a group of 2-3.

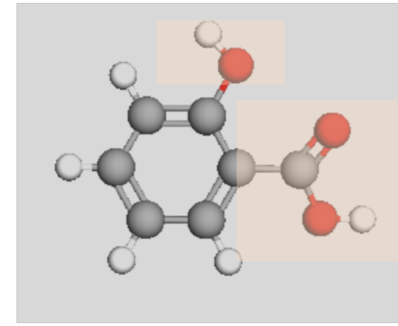
Synthesis of Aspirin



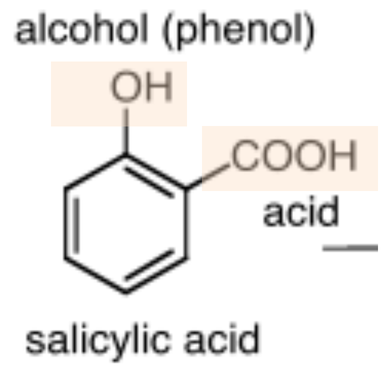


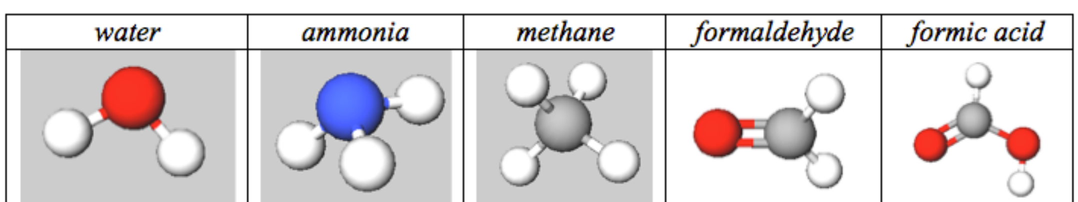
REACTANT: Salicylic Acid

Common Functional Groups



Name	General Formula
Alcohols	R–OH
Ethers	R–O–R′
Amines	$R-NH_2$
Carboxylic Acids	$R\text{-}\overset{\overset{\displaystyle O}{\|}}{C}\text{-}OH$

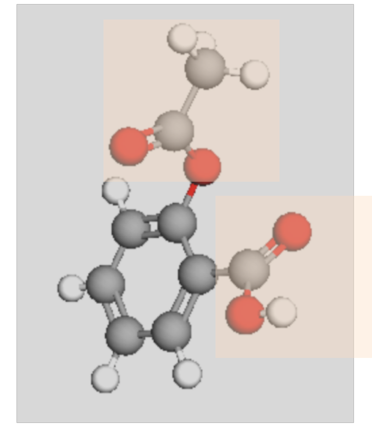


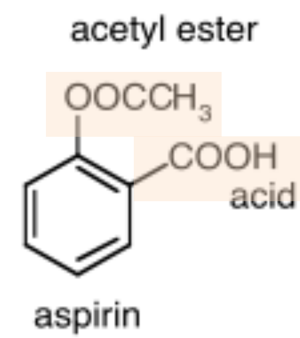


PRODUCT: Acetyl salicylic acid (aspirin)

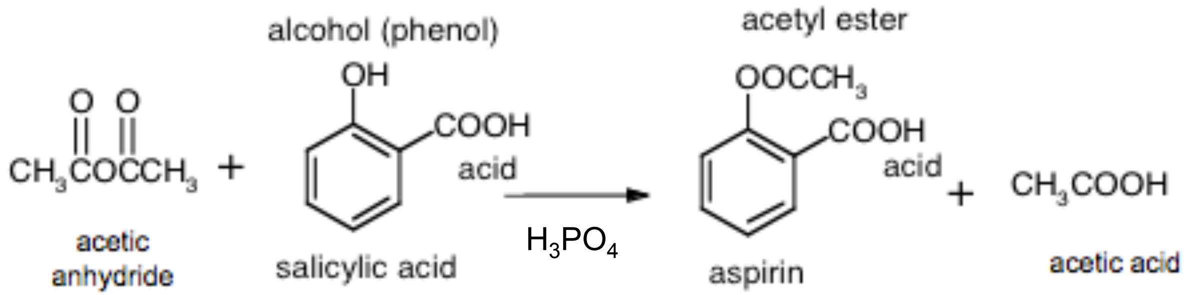
Common Functional Groups

Name	General Formula
Aldehydes	R-C(=O)-H
Ketones	R-C(=O)-R'
Carboxylic Acids	R-C(=O)-OH
Esters	R-C(=O)-OR'
Amides	R-C(=O)-N(R')(R'')





Synthesis of Aspirin



1. **Get equipment from stockroom with your group.**
2. **Follow instructions in lab manual carefully. Be mindful of your safety. WEAR eye protection.**

3. **Store in lab drawer as instructed in Part A.3 of the instructions of the lab procedure.**

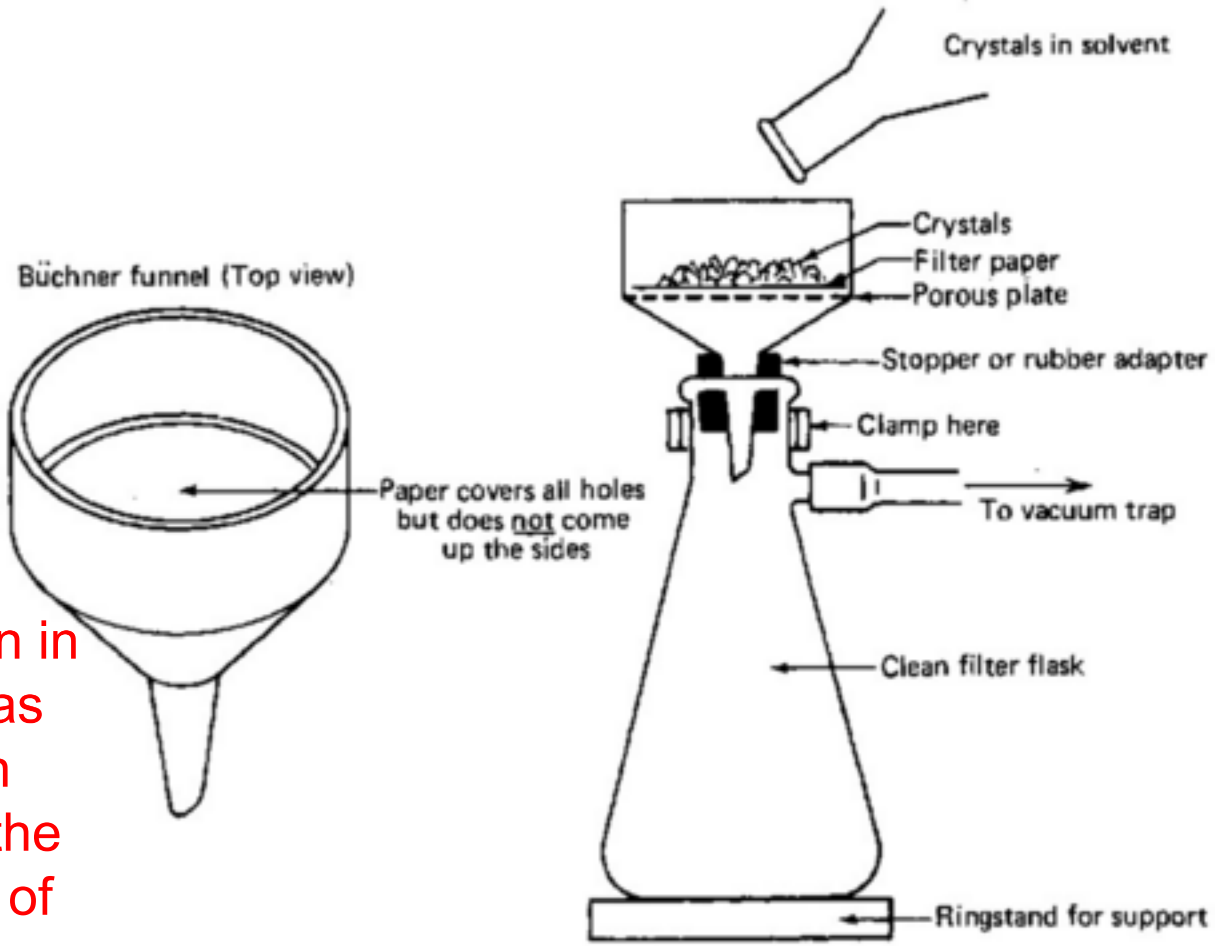
Equipment

From the stockroom:
- Beaker clamp
- filter flask
- Büchner funnel
- ice bath – in lab

From the common drawer:
- ring stand and ring
- wire gauze
- Bunsen burner

From your drawer:
- 125 mL Erlenmeyer flask
- large beaker

Vacuum Filtration

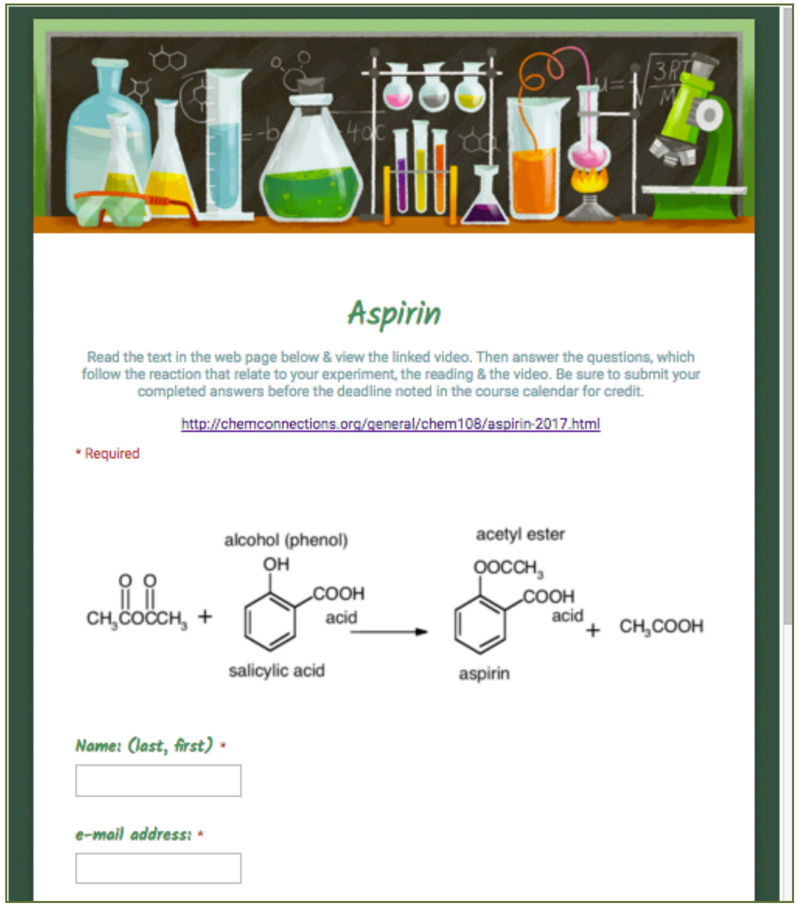


Store aspirin in lab drawer as instructed in Part A.3 of the instructions of the lab procedure.

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

Completed Report Form & On-line Post Lab Due next week.

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


Aspirin

Read the text in the web page below & view the linked video. Then answer the questions, which follow the reaction that relate to your experiment, the reading & the video. Be sure to submit your completed answers before the deadline noted in the course calendar for credit.

http://chemconnections.org/general/chem108/aspirin-2017.html

* Required

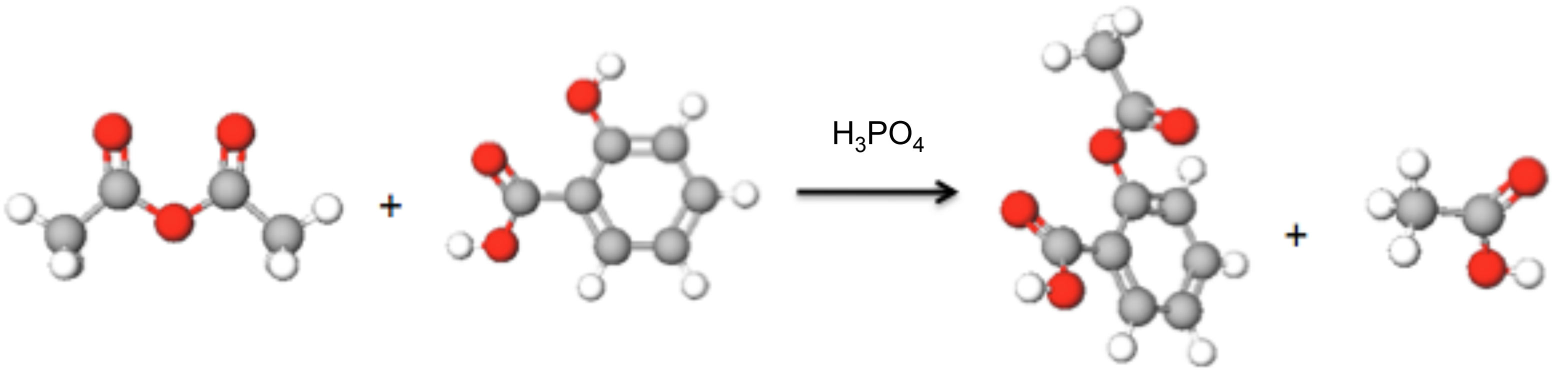
Name: (last, first) *

e-mail address: *

Store filtered crude aspirin in lab drawer and weigh next week.

NEXT WEEK: Calculate % Yield.

TODAY: *Calculate Theoretical Yield*



grams (Salicylic Acid) → grams (Aspirin)

Using Mass of salicylic acid from page 90.

Moles

Molar Mass

Stoichiometry

$C_9H_8O_4$

MW = 180.15

? grams (SA)	1 mol (SA)	1 mol A	grams (A) (Molecular Weight A)
	grams (SA) (Molecular Weight SA)	1 mol SA	1 mol (A)

= ? (A)

"Gatekeeper"

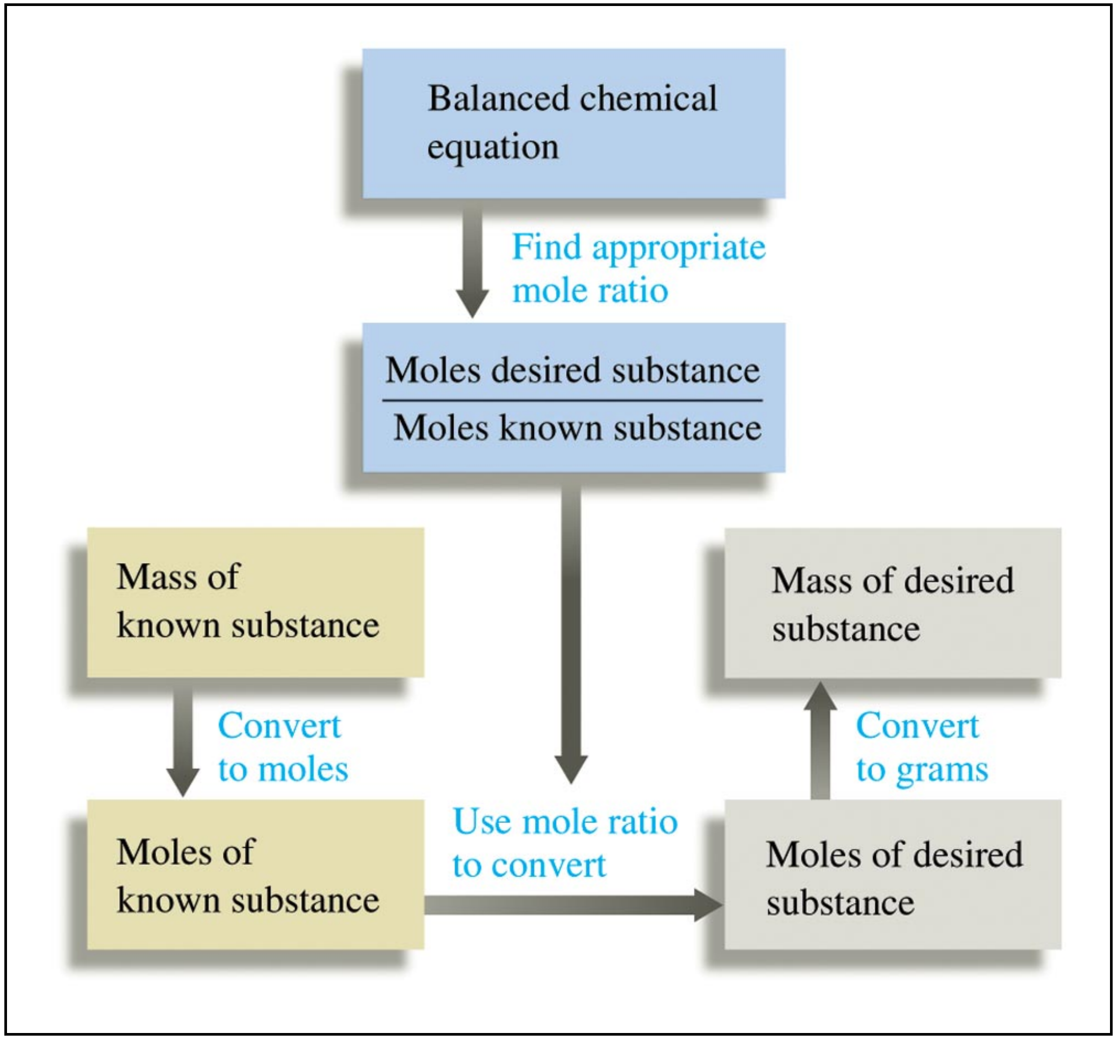
$C_7H_6O_3$

MW = 138.12

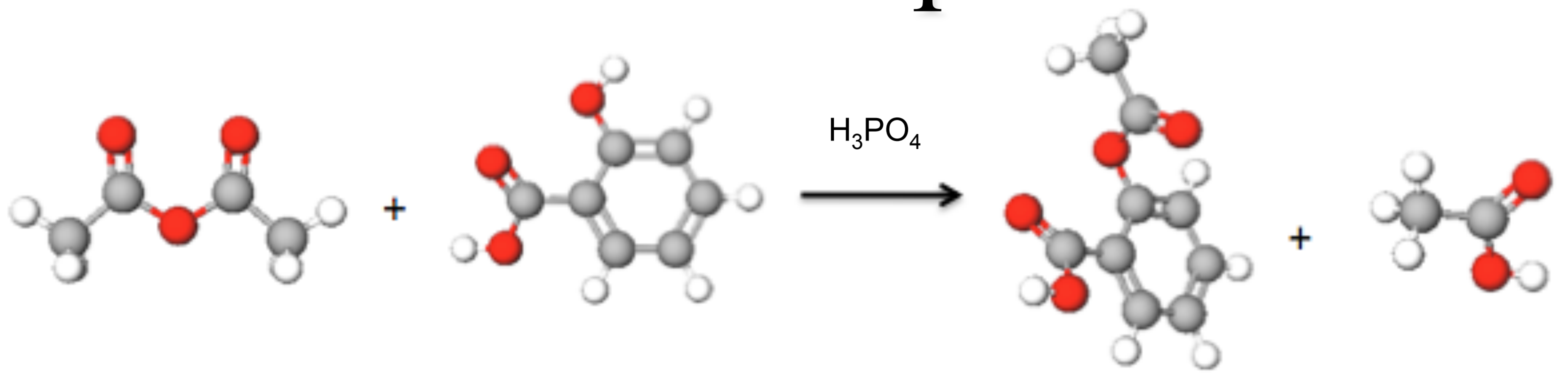
???

aspirin

Mass Calculations: Reactants ⟷ Products



Example



grams (Salicylic Acid) → grams (Aspirin)

Moles

Molar Mass

Stoichiometry

$C_9H_8O_4$

MW = 180.15

5.0 grams (SA)	1 mol (SA)	1 mol A	grams (A) (Molecular Weight A)	= ? (A)
	grams (SA) (Molecular Weight SA)	1 mol SA	1 mol (A)	

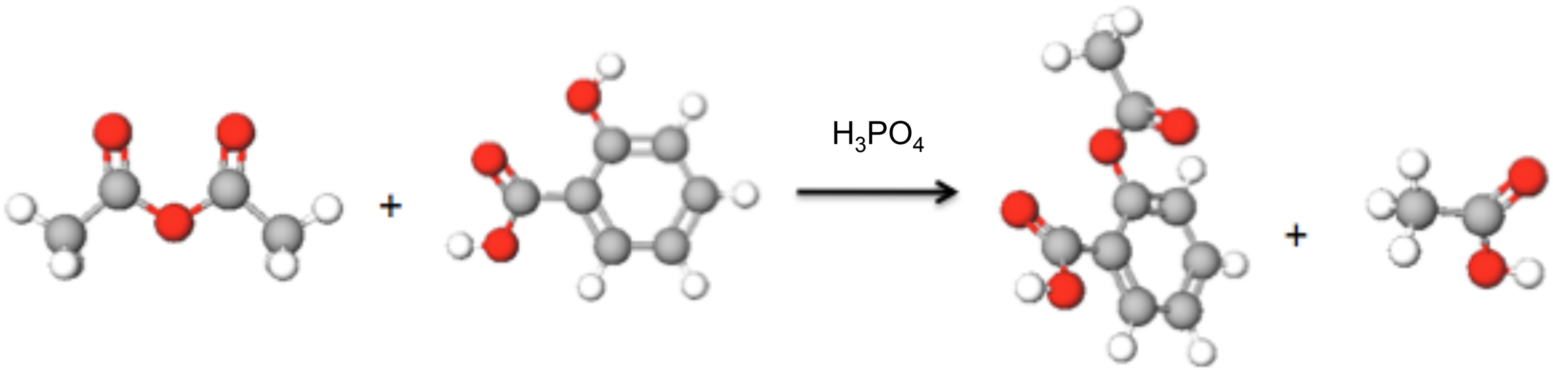
"*Gatekeeper*"

$C_7H_6O_3$

MW = 138.12

6.5 g aspirin

TODAY: *Calculate Theoretical Yield*



grams (Salicylic Acid) → grams (Aspirin)

Moles
Molar Mass
Stoichiometry

Using your mass of salicylic acid from page 90.

$C_9H_8O_4$
MW = 180.15

? grams (SA)	1 mol (SA)	1 mol A	grams (A) (Molecular Weight A)	= ? (A)
	grams (SA) (Molecular Weight SA)	1 mol SA	1 mol (A)	

"Gatekeeper"

$C_7H_6O_3$
MW = 138.12

???
aspirin

Show clearly labeled calculation with units & correct s.f ; Have pg. 90 signed before leaving lab.

Percent Yield

- In synthesis as in any experiment, it is very difficult and at most times impossible to be perfect. Therefore the actual yield (g) is measured and compared to the theoretical calculated yield (g). This is the percent yield:

- % Yield = actual (g) / theoretical (g) x 100

This calculation is for next week.