Organic Molecules

Structures, Functional Groups, Reactions

Dr. Ron Rusay

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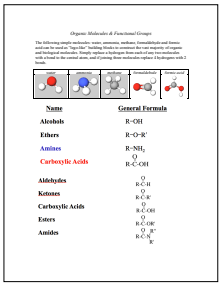
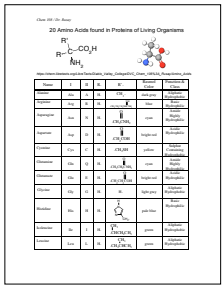
Functional Groups & Amino Acids



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 of course those molecules replace 2 hydrogens with 2 bonds.

Name	General Formula
Alcohols	R–OH
Ethers	R–O–R'
Amines	$R–NH_2$
Carboxylic Acids	O ‖ R-C-OH
Aldehydes	O ‖ R-C-H
Ketones	O ‖ R-C-R'
Carboxylic Acids	O ‖ R-C-OH
Esters	O ‖ R-C-OR'
Amides	O R'' \ / R-C-N / \ R'



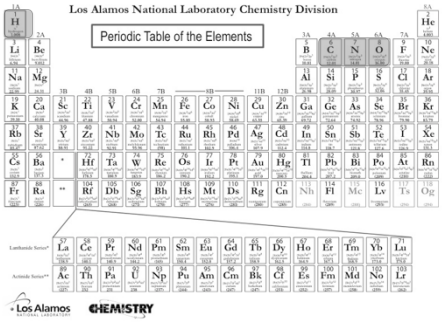
Chem 108 / Dr. Rusay

20 Amino Acids found in Proteins of Living Organisms

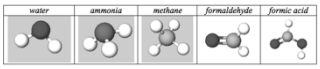
https://www.chemistry.wustl.edu/~biochem/courses/_temp_dir/tmp2b1C_Chem_108/b2b_Young/Amino_Acids

Name	1	2	3	R	Polarity Charge	Hydrophobicity Class
Glycine	Gly	G	Gly	H	non-polar	Amphipathic (Neutral)
Alanine	Ala	A	Ala	CH_3	non-polar	Hydrophobic
Arginine	Arg	R	Arg	$CH_2CH_2CH_2NH-C(=NH_2)^+-NH_2$	base	Amphipathic (Hydrophilic)
Asparagine	Asn	N	Asn	CH_2CONH_2	polar	Amphipathic (Hydrophilic)
Aspartate	Asp	D	Asp	CH_2COO^-	negatively charged	Amphipathic (Hydrophilic)
Cysteine	Cys	C	Cys	CH_2SH	polarizable	Amphipathic (Contains Sulfur)
Glutamate	Glu	E	Glu	$CH_2CH_2COO^-$	polar	Amphipathic (Hydrophilic)
Glutamate	Gln	Q	Gln	$CH_2CH_2CONH_2$	negatively charged	Amphipathic (Hydrophilic)
Glycine	Gly	G	Gly	H	non-polar	Amphipathic (Hydrophobic)
Histidine	His	H	His		polar base	Basic (Hydrophilic)
Isoleucine	Ile	I	Ile	$CH(CH_3)CH_2CH_3$	polar	Amphipathic (Hydrophobic)
Leucine	Leu	L	Leu	$CH_2CH(CH_3)_2$	polar	Amphipathic (Hydrophobic)

Elemental building blocks for all organic molecules



Organic Molecules



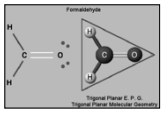
Shapes, Functions & Structural Analogies

Water, Ammonia, Methane

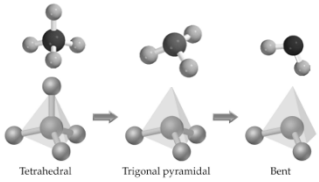
Plus >C=O "carbonyls"

Molecular Models for C, H, N, O

Fundamental repeating shapes found in every biological molecule



C =black
H = gray
N = blue
O = oxygen



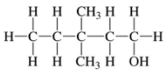
pink = generic atom

Representing Organic Molecules

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

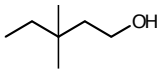
Representing Organic Molecules
Common Formulas & Drawings

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



Condensed Structure:
$CH_3CH_2C(CH_3)_2CH_2CH_2OH$ or $CH_3CH_2\overset{CH_3}{\underset{CH_3}{C}}CH_2CH_2OH$

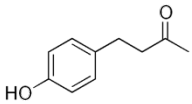
Bond-Line Structure:

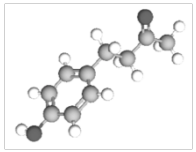


QUESTION

A compound that smells like fresh raspberries, the following structure, $C_?H_?O_?$, matches its calculated molar mass which is 164 g/mol.

A) TRUE
B) FALSE

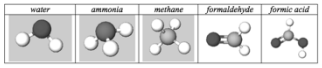




Organic Molecules
Common Functional Groups

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

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



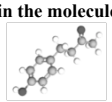
Organic Molecules
Common Functional Groups

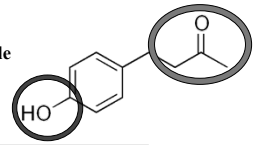
Name	General Formula
Aldehydes	R-C(=O)-H
Ketones	R-C(=O)-R'
Carboxylic Acids	R-C(=O)-OH
Esters	R-C(=O)-OR'
Amides	R-C(=O)-N(R")R'

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

QUESTION

Select the function(s) in the molecule

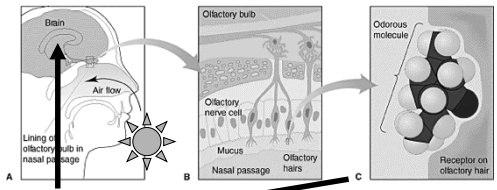




	Alcohol	R−OH
	Ether	R−O−R′
	Amine	R−NH_2
	Aldehyde	R-C(=O)-H
	Ketone	R-C(=O)-R'
	Carboxylic Acid	R-C(=O)-OH
	Ester	R-C(=O)-OR'
	Amide	R-C(=O)-N(R")R'

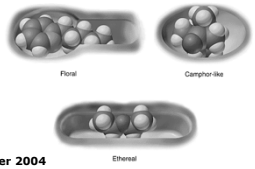
Detecting stuff we cannot see: the Sense of Smell
Models, Theories & Interactions

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



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

Historical view of a few smell receptors.



4 October 2004

The Nobel Assembly at Karolinska Institutet has today decided to award

The Nobel Prize in Physiology or Medicine for 2004

jointly to

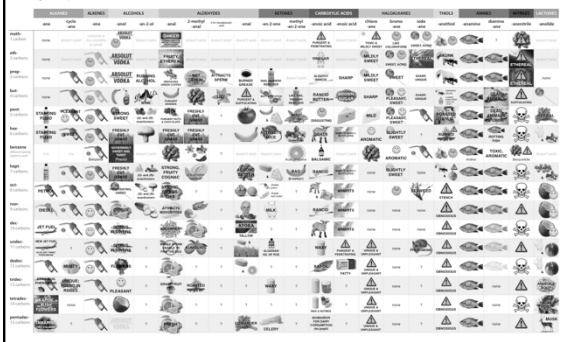
Richard Axel and Linda B. Buck

for their discoveries of

"odorant receptors and the organization of the olfactory system"

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

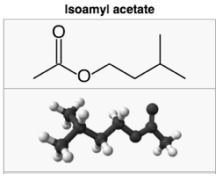
Organic Functions & Smell Receptors.

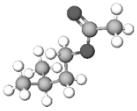


One molecule, one function: One Smell Receptor

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

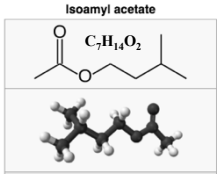




$C_7H_{14}O_2$

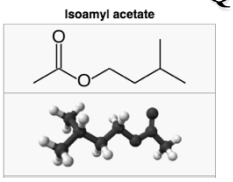
One molecule among 82 primary chemicals found in bananas:

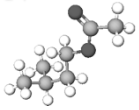
Isoamyl acetate



QUESTION

Isoamyl acetate





$C_7H_{14}O_2$

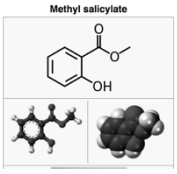
The function in isoamyl acetate's structure is a(n):

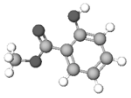
A.Alcohol
B.Aldehyde
C.Ketone
D.Ester
E.Carboxylic Acid

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

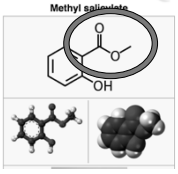


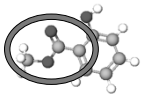


$C_8H_8O_3$

QUESTION

Methyl salicylate





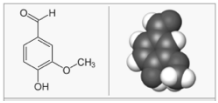
$C_8H_8O_3$

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 ~ $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 (2×10^{-11} g per 1,000 cm^3 of air).

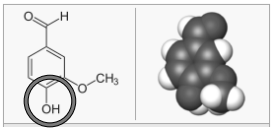
Vanillin

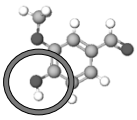


Bonus:
The space (volume) of the Oakland Coliseum Arena, aka Oracle Arena, is approximately 90,000,000 ft^3. If 1.00g of the compound were released at center court, and was completely and evenly dispersed throughout the building, would you smell it sitting in sec. 204, row H, seat 121? Show your calculation.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

QUESTION

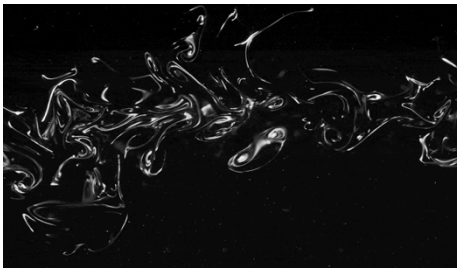
Vanillin





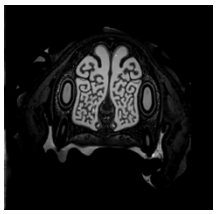
One of the functions, an alcohol, is circled. What are the other two functions?:
A.Aldehyde + Ketone
B.Carboxylic Acid + Ester
C.Ketone + Ether
D.Aldehyde + Ether
E.Carboxylic Acid + Aldehyde

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

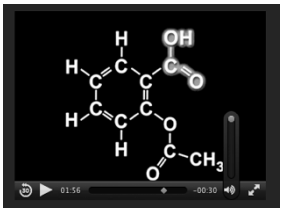


https://www.youtube.com/watch?v=FLH36ML8IEU

Dogs Can Smell Cancer - Secret Life of Dogs - BBC

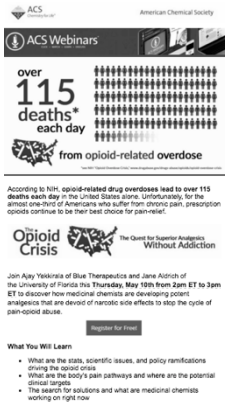
https://www.youtube.com/watch?v=e0UK6kkS0_M

Synthesis of a Non-steroid anti-inflammatory drug Aspirin

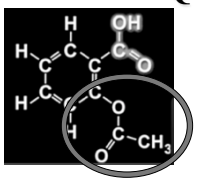


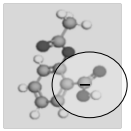
http://chemconnections.org/general/movies/Representations.MOV

Synthesis of a Non-steroid anti-inflammatory drug Aspirin & Pain



QUESTION

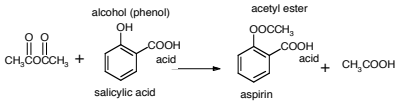


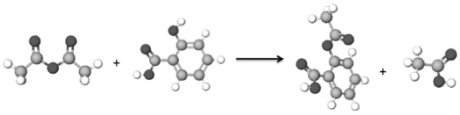


One of aspirin's functions, an ester, is circled in blue. What is the highlighted yellow function?:

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

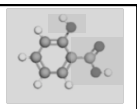
Synthesis of Aspirin





Salicylic Acid

Common Functional Groups



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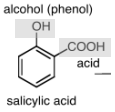
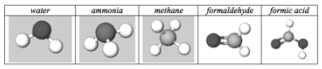
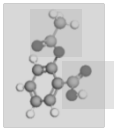
Amines	
Carboxylic Acids	R-C(=O)-OH





Aspirin

Common Functional Groups



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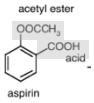
Ketones	R-C(=O)-R'
Carboxylic Acids	R-C(=O)-OH
Esters	R-C(=O)-OR'
Amides	R-C(=O)-N(R")-R'



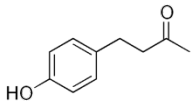
Discussion Questions

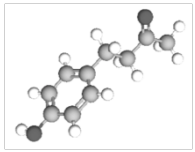
http://chemconnections.org/general/chem108/Organic%20Chemistry%20Guide.html

QUESTION

A compound that smells like fresh raspberries, the following structure, $C_?H_?O_?$, matches its calculated molar mass which is 164 g/mol.

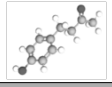
A) TRUE
B) FALSE

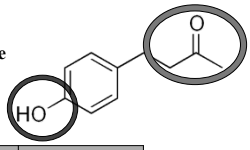




QUESTION

Select the function(s) in the molecule

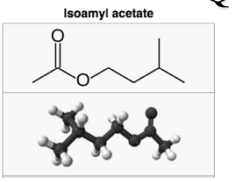


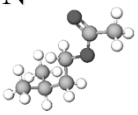


	Alcohol	R−OH
	Ether	R−O−R′
	Amine	$R-NH_2$
	Aldehyde	R-C(=O)-H
	Ketone	R-C(=O)-R'
	Carboxylic Acid	R-C(=O)-OH
	Ester	R-C(=O)-OR'
	Amide	R-C(=O)-N(R")-R'

QUESTION

Isoamyl acetate



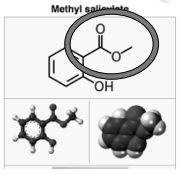


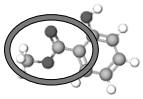
$C_7H_{14}O_2$

The function in isoamyl acetate's structure is a(n):
A.Alcohol
B.Aldehyde
C.Ketone
D.Ester
E.Carboxylic Acid

QUESTION

Methyl salicylate



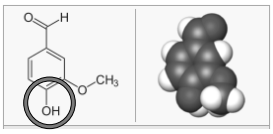


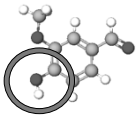
$C_8H_8O_3$

One of the functions, an ester, is circled. What is the other function?:
A.Alcohol
B.Ether
C.Ketone
D.Aldehyde
E.Carboxylic Acid

QUESTION

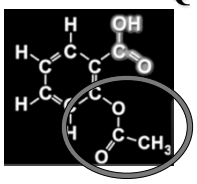
Vanillin

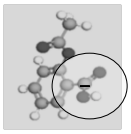




One of the functions, an alcohol, is circled. What are the other two functions?:
A.Aldehyde + Ketone
B.Carboxylic Acid + Ester
C.Ketone + Ether
D.Aldehyde + Ether
E.Carboxylic Acid + Aldehyde

QUESTION



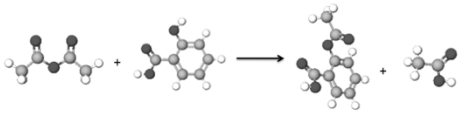


One of aspirin's functions, an ester, is circled in blue. What is the highlighted yellow function?:

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

QUESTION

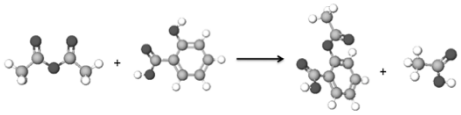
- **How many grams of aspirin can be theoretically produced from 5.0 g of salicylic acid reacting with an excess of acetic anhydride, $C_4H_6O_3$?**
- **Balanced Equation:**



	salicylic acid	aspirin	
$C_4H_6O_3$	$C_7H_6O_3$	$C_9H_8O_4$	$C_2H_4O_2$
MW = 102.09	MW = 138.12	MW = 180.15	MW= 60.05

A) 3.8 g B) 5.0 g C) 6.5 g D) 7.8 g

Mass Calculations:



grams (Salicylic Acid) ⟶ grams (Aspirin)

Moles
Molar Mass
Stoichiometry

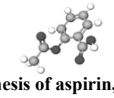
$C_9H_8O_4$
MW = 180.15

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

$C_7H_6O_3$
MW = 138.12

A) 3.8 g B) 5.0 g C) 6.5 g D) 7.8 g

QUESTION



✿ **Kaitlyn's synthesis of aspirin, $C_9H_8O_2$, 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%