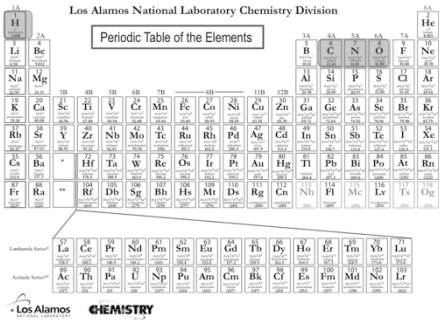
Organic Molecules

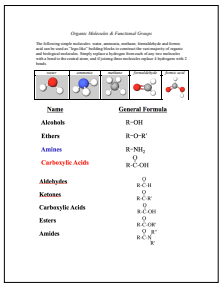
Functional Group Overview

Dr. Ron Rusay

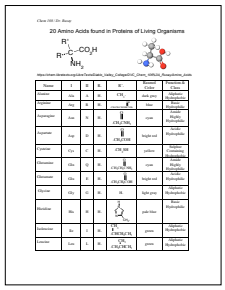
Elemental building blocks for all organic molecules



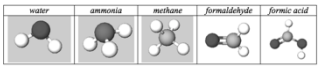
Functional Groups & Amino Acids



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″)



Organic Molecules



Shapes, Functions & Structural Analogies

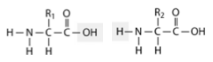
Water, Ammonia, Methane

Plus >C=O "carbonyls"

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

Amines $R–NH_2$

Carboxylic Acids R–C(=O)–OH



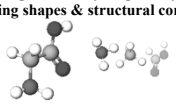
	Functions	
	Alcohol	R–OH
	Ether	R–O–R′
X	Amine	$R–NH_2$
	Aldehyde	R–C(=O)–H
	Ketone	R–C(=O)–R′
X	Carboxylic Acid	R–C(=O)–OH
	Ester	R–C(=O)–OR′
	Amide	R–C(=O)–N(R′)(R″)

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

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 structures for the chemistry of life.

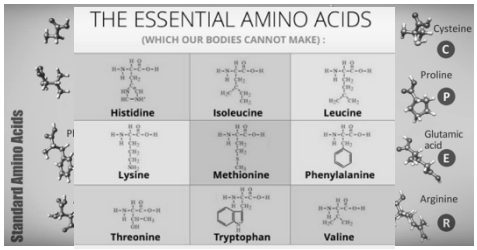
•There are less than 20,000 total proteins produced from humans' entire genome, each coded by a specific gene in DNA's ~3 billion genetic bases.

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

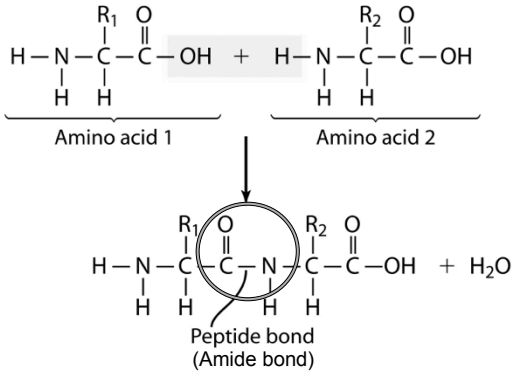
Amino Acids

Legos of Chemical Biology

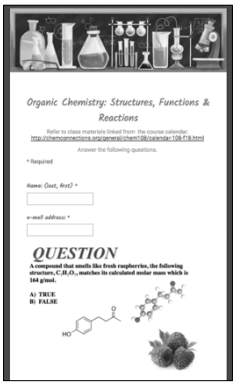
All amino acids contain C, H, O, and N; two, C & M. also have sulfur.



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



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

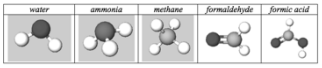


Organic Molecules

Common Functional Groups

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

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



Organic Molecules

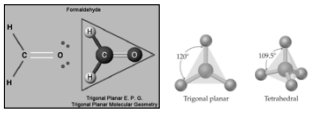
Common Functional Groups

Name	General Formula
Aldehydes	$R-\overset{O}{\overset{\|}{C}}-H$
Ketones	$R-\overset{O}{\overset{\|}{C}}-R'$
Carboxylic Acids	$R-\overset{O}{\overset{\|}{C}}-OH$
Esters	$R-\overset{O}{\overset{\|}{C}}-OR'$
Amides	$R-\overset{O}{\overset{\|}{C}}-\overset{R''}{\underset{R'}{N}}$

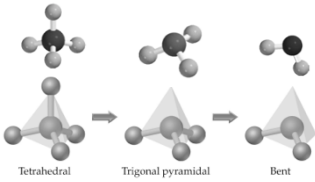
R′− or R− represents any generic carbon atom bonded in the functional group

Molecular Models for C, H, N, O

Fundamental repeating shapes found in every biological molecule



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



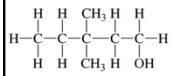
pink = generic atom

Representing Organic Molecules

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

Representing Organic Molecules
Common Formulas & Drawings

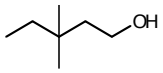
Molecular formula: $C_7H_{16}O$ **Empirical Formula:** $C_7H_{16}O$



Condensed Structure:

$CH_3CH_2C(CH_3)_2CH_2CH_2OH$ or $CH_3CH_2\underset{\displaystyle CH_3}{\overset{\displaystyle CH_3}{C}}CH_2CH_2OH$

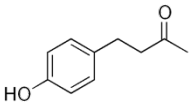
Bond-Line Structure:

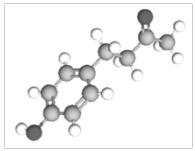


QUESTION

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



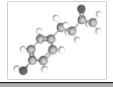


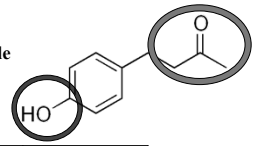
Organic Chemistry: Structures, Functions & Reactions

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

QUESTION

Select the function(s) in the molecule

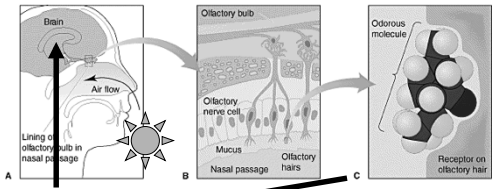




	Alcohol	R−OH
	Ether	R−O−R′
	Amine	$R-NH_2$
	Aldehyde	
	Ketone	
	Carboxylic Acid	
	Ester	
	Amide	

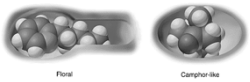
Detecting stuff we cannot see: the Sense of Smell
Models, Theories & Interactions

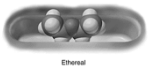
http://chemconnections.org/organic/chem226/Labs/Smell/smell-links.html



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

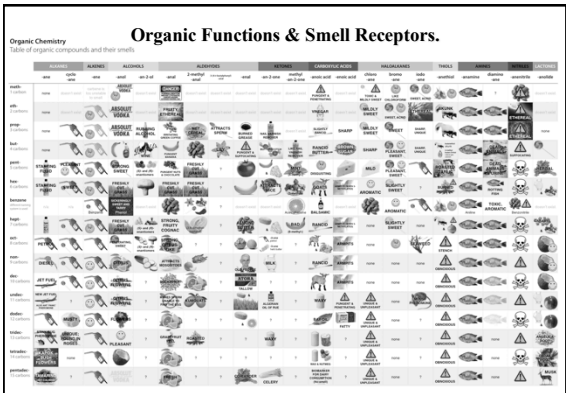
Richard Axel and Linda B. Buck

for their discoveries of

"odorant receptors and the organization of the olfactory system"

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

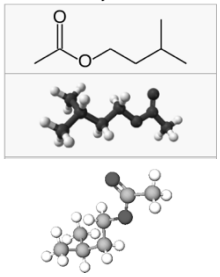
Organic Functions & Smell Receptors.



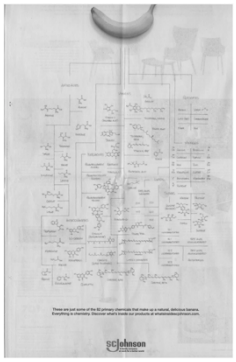
One molecule, one function: One Smell Receptor

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

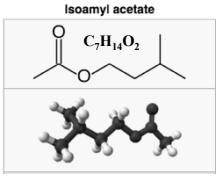


$C_7H_{14}O_2$



One molecule among 82 primary chemicals found in bananas:

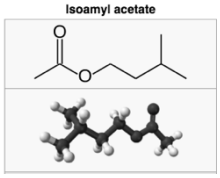
Isoamyl acetate

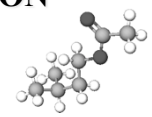


$C_7H_{14}O_2$

QUESTION

Isoamyl acetate





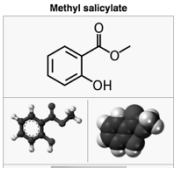
$C_7H_{14}O_2$

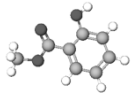
The function in isoamyl acetate's structure is a(n):
A.Alcohol
B.Aldehyde
C.Ketone
D.Ester
E.Carboxylic Acid

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

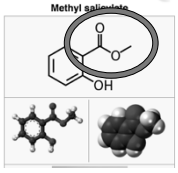




$C_8H_8O_3$

QUESTION

Methyl salicylate



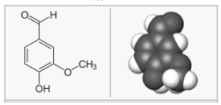
$C_8H_8O_3$

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).

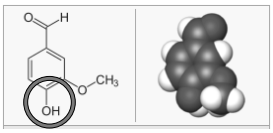
Vanillin

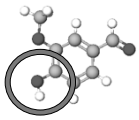


Bonus:
The space (volume) of the Oakland Coliseum Arena, aka Oracle Arena, is approximately 90,000,000 ft^3. If 1.00g of the compound were released at center court, and was completely and evenly dispersed throughout the building, would you smell it sitting in sec. 204, row H, seat 121? Show your calculation.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

QUESTION

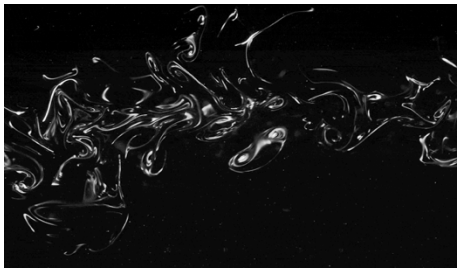
Vanillin





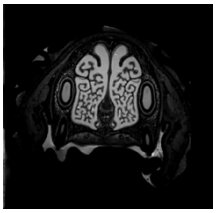
One of the functions, an alcohol, is circled.
What are the other two functions?:
A.Aldehyde + Ketone
B.Carboxylic Acid + Ester
C.Ketone + Ether
D.Aldehyde + Ether
E.Carboxylic Acid + Aldehyde

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

Name: _____

Organic Functional Group Sudoku Puzzle
adapted from
Crute, Thomas D.; Myers, Stephanie A., *J. Chem. Educ.* 2007, 84, 612

The presence of the sudoku puzzle was first published in the United States in 1979 by Howard Garns, a retired architect and freelance puzzle constructor. In April 1984, the puzzle was introduced in Japan and the name "sudoku" was assigned to the puzzle. "Suuji wa dokushin ni kagiru" may be translated as "the numbers must be single" or "the numbers must occur only once". Later the name was abbreviated to sudoku (pronounced SOU-dough-coo, "su" means number, "doku" means single). In April 2005, The *New York Post* published sudoku puzzles as a regular feature and by July 2005, the puzzle surged in popularity all over the country (1, 2).

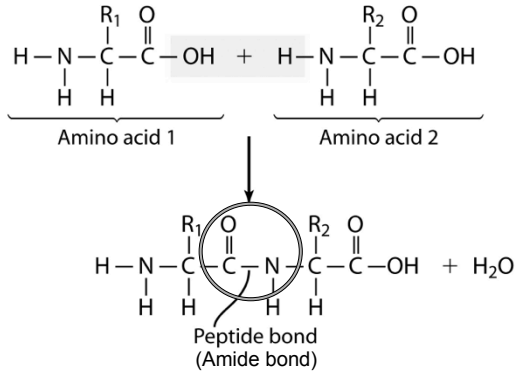
The following Sudoku puzzle deals with the names and generic structures of organic functional groups found in organic molecules. They do not deal directly with numbers as

	R-COOH					$R\text{-}CONH_2$	$R\text{-}NH_2$	R-CO-R´
$R\text{-}NH_2$	R-Cl	R-CO-R´	R-OH			R-O-R´		
R-O-R´					R-COO-R´		R-Cl	R-OH
R-CO-R´								
R-COO-R´	R-OH		R-O-R´	$R\text{-}NH_2$	R-CO-R´		R-COOH	$R\text{-}CONH_2$
								R-O-R´
$R\text{-}CONH_2$	R-CO-R´		R-COOH					R-Cl
		$R\text{-}NH_2$			R-Cl	R-OH	$R\text{-}CONH_2$	R-COO-R´
R-Cl	R-COO-R´	R-CHO					R-O-R´	

Organic Molecules
Functional Groups

Proteins
Amines, Carboxylic Acids
Amides (Peptides)

Physiological reactions (metabolism) of one gram of protein produces 4 to 5 Calories (kcal), which is enough energy to raise the water in your body about 1 °C.



Proteins: Macromolecular Biopolymers

- **Structural proteins:** ***Collagen***
  ***Connectin proteins*, β - MW of 2.1 million g/mol; length = 1000 nm; can stretch to 3000 nm.**
- **Mechanical (Contractile) proteins: *Actin, Myosin***
- **Transport proteins: *Hemoglobin***
- **Enzymes: *Glutamine synthetase* - 12 subunits of 468 residues each; total mol. wt. = 600,000 daltons**
- **Regulatory proteins: *Insulin* - α -alpha chain of 21 residues, β - beta chain of 30 residues; total mol. wt. of 5,733 amu**
- **Specialized proteins: *Antifreeze in fish***

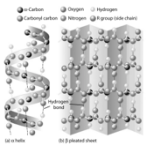
A gene was first defined as: one piece of DNA that codes for one protein. (The definition is being expanded beyond proteins to include certain types of RNA.)

Proteins: Macromolecular Biopolymers

Examples of Structural Proteins

Collagen: connective tissue

Structural Proteins:
Silk

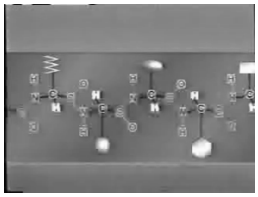


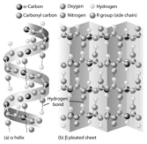
β-Sheets

http://chemconnections.org/general/movies/proteins-silk-2.mov

Structural Proteins:

α-Helix
Curly Hair

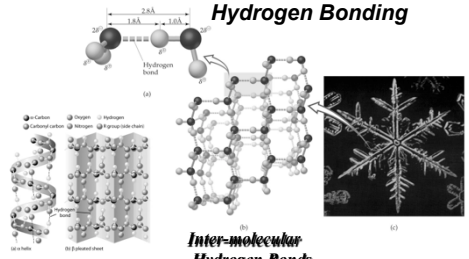




http://chemconnections.org/general/movies/protein-hair-2.mov
Annenberg World of Chemistry
#23 Proteins : *http://www.learner.org/resources/series61.html*

Intra- & Inter-molecular

Hydrogen Bonding



Inter-molecular Hydrogen Bonds

α-Helix β-Sheets

Intra-molecular Hydrogen Bonds

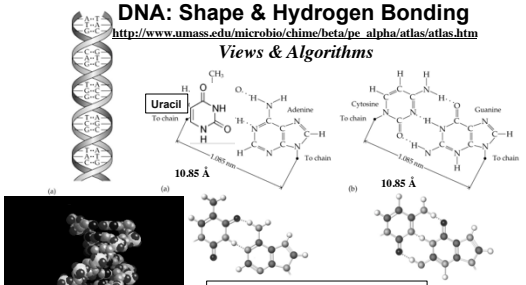
http://chemconnections.org/general/movies/ice-structure.MOV

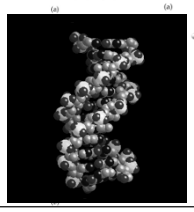
http://chemconnections.org/general/movies/HydrogenBonding.MOV

DNA: Shape & Hydrogen Bonding

http://www.umass.edu/microbio/chime/beta/pe_alpha/atlas/atlas.htm

Views & Algorithms

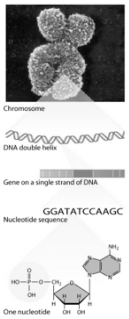




Chemical Biology

DNA ⇆ RNA ⇆ Proteins

Uracil



https://www.youtube.com/watch?v=gG7uCskUOrA

Chemical Biology

DNA ⇆ RNA ⇆ Proteins

https://www.youtube.com/watch?v=X_tYrnv_o6A

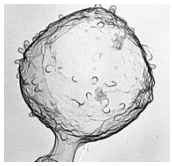
Mechanical proteins:

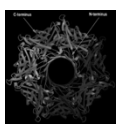
Pathogens & Cell Invasion

http://chemconnections.org/organic/chem226/Announcements-info/Staph-infection/infection.html

myosin-actin: muscle

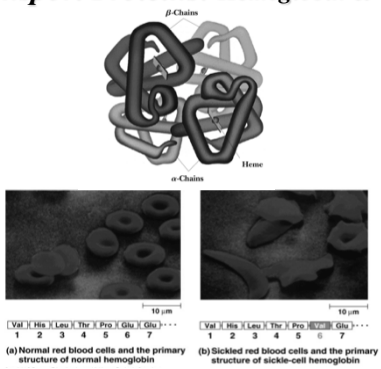
Michael Ferenczi



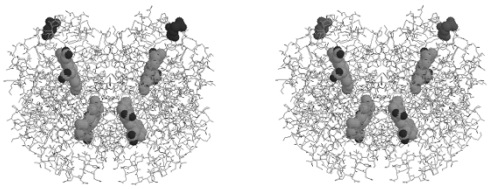


Streptococcus pyogenes
96,000 x
Vincent A. Fischetti Ph.D., Rockefeller University
http://www.chm.bris.ac.uk/motm/motm.htm

Transport Proteins: ***Hemoglobin & Oxygen***



Normal hemoglobin vs sickle cell hemoglobin



Valine replaces Glutamate

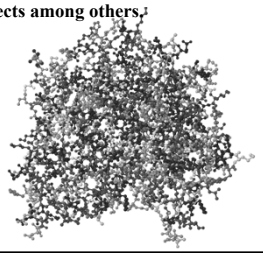
http://chemconnections.org/Presentations/Columbia/slide8-3.html

Firefox to listen

Catalytic Proteins: Enzymes

Acetylcholinesterase (ACE)

***ACE*, an enzyme, which catalyzes a key reaction in a repetitive biochemical cycle that is crucial to neurological and physiological functions in humans…. and insects among others.**



4,496 atoms;
4,404 bonds
574 amino acid residues

Protective Proteins

Immunoglobin

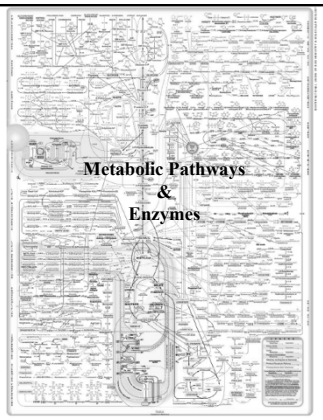
Antibodies

Prolific Immunoproteins

Human's total ~ 100 x 10 ^{6} immunoproteins

Combinatorial syntheses from libraries of 250, 10, and 6 possible contributors

Human Genome ~20,000 proteins



Metabolic Pathways
&
Enzymes

Name: _____

Organic Functional Group Sudoku Puzzle
adapted from
Crute, Thomas D.; Myers, Stephanie A., *J. Chem. Educ.* 2007, 84, 612

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The following Sudoku puzzle deals with the names and generic structures of organic functional groups found in organic molecules. There do not deal directly with numbers as

	R-COOH					R-$CONH_2$	R-NH_2	R-CO-R′
R-NH_2	R-Cl	R-CO-R′	R-OH			R-O-R′		
R-O-R′					R-COO-R′		R-Cl	R-OH
R-CO-R′								
R-COO-R′	R-OH		R-O-R′	R-NH_2	R-CO-R′		R-COOH	R-$CONH_2$
								R-O-R′
R-$CONH_2$	R-CO-R′		R-COOH					R-Cl
		R-NH_2			R-Cl	R-OH	R-$CONH_2$	R-COO-R′
R-Cl	R-COO-R′	R-CHO					R-O-R′	

Organic Molecules

Functional Groups

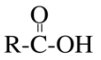
alcohols, ethers, aldehydes, ketones

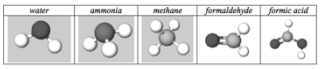
Carbohydrates / Saccharides / Sugars

Physiological reactions (metabolism) of one gram of carbohydrate produces about the same energy as 1 gram of protein: 4 to 5 Calories (kcal); enough to raise the water in your body about 1 ºC.

Sugars (Carbohydrates)

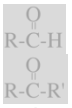
Common Functional Groups

Name	General Formula
Alcohols	R–OH
Ethers	R–O–R′
Amines	R–NH_2
Carboxylic Acids	



Sugars (Carbohydrates)

Common Functional Groups

Name	General Formula
Aldehydes	
Ketones	
Carboxylic Acids	
Esters	
Amides	

Carbohydrate ("-ose") Formation

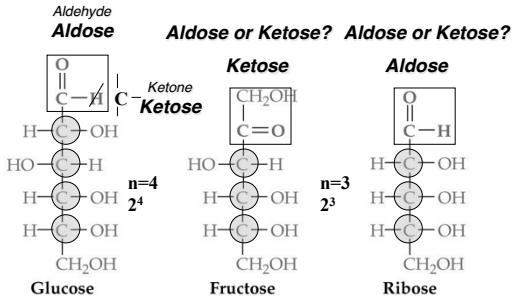
Photosynthesis

Light + chlorophyll an + two greenhouse gases, which provide oxygen & sugars

$$n\,CO_2 + n\,H_2O \longrightarrow C_n(H_2O)_n + n\,O_2$$

- **Empirical formula = CH_2O**
- **Monosaccharides (simple sugars)**
- **C_5 : pent-oses – *rib-ose***
- **C_6 : hex-oses – *fruct-ose, gluc-ose***

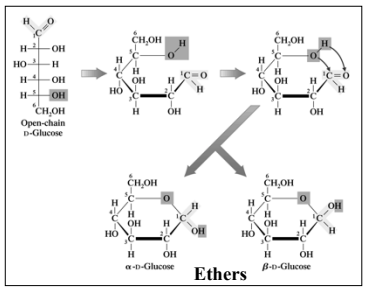
Can be either an ald-ose (aldehyde + alcohols) or ket-ose (ketone + alcohols)



There are 2^n possible stereoisomers, where n = the number of chiral atoms (alcohols). Glucose? Fructose? Ribose?

Plus the cyclized forms of each of the sixteen, which adds a chiral carbon, D-Glucose for example:

D-glucose can cyclize intramolecularly



Ethers

Sugar Wordsearch

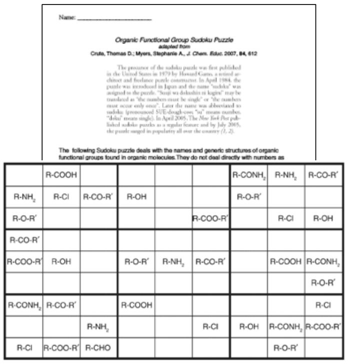
Terry L. Helser
Department of Chemistry, SUNY College at Oneonta, Oneonta, NY 13820-4015; *helsert@oneonta.edu*

This puzzle contains 29 names, terms, prefixes, and acronyms that describe sugars and their polymers. Find and highlight these terms in the matrix below. "CARBOHYDRATE" is already done for you. Then, correctly transfer them to the blanks in the description below the matrix. Use the letters remaining in the matrix to complete the sentence describing these molecules. Your success will be rewarded. The answers to the Sugar Wordsearch are found below. Good hunting!

```
N I E T O R P O C Y L G S U
N I T I H C G L U C O S E G
K E T O S E S S E S O D L A
E A G C H E X O S E I P E R
S S L S E S O B I R A Y S S
O U Y T M P A M A M K R O N
T G C A R B O H Y D R A T E
C A O R E N C L L I F N C G
A R L C O C O E Y S W O U O
L N I H A S E L P M I S R C
A A P S E R E M O N A E F Y
G N I C U D E R E T S E E L
E D D C E L L U L O S E T G
```

CARBOHYDRATEs can be S_____ S_____s that are either A_____ or K_____ and are therefore R_____ sugars. Table sugar, S_____, is a D_____ of the H_____s F_____ and G_____, in cyclic furanose and P_____ forms, respectively. I_____ is glucose linked to G_____. Plants store energy in the ____saccharide S_____, which contains A_____ and A_____. The animal equivalent is G_____. The only ____mer in them is the alpha A_____ of glucose. Beta-linked glucose or *N*-acetylglucosamine makes C_____ or C_____, respectively. Both are structural polymers. Complex molecules like G_____s and _____P_____s have sugars attached. Finally, phosphodi_____ bonds link R_____ units in the backbone of ____. Converting the pentose into the deoxy form produces a ___ strand.

Use the remaining letters to fill in the following sentence: _____ _____ _____ _____



Name: ______________________

Organic Functional Group Sudoku Puzzle
adapted from
Crute, Thomas D.; Myers, Stephanie A., *J. Chem. Educ.* 2007, 84, 612

The precursor of the sudoku puzzle was first published in the United States in 1979 by Howard Garns, a retired architect and freelance puzzle constructor. In April 1984, the puzzle was introduced in Japan and the name "sudoku" was assigned to the puzzle. "Suuji wa dokushin ni kagiru" may be translated as "the numbers must be single" or "the numbers must occur only once". Later the name was abbreviated to sudoku (pronounced SUE-dough-coo; "su" means number, "doku" means single). In April 2005, The *New York Post* published sudoku puzzles as a regular feature and by July 2005, the puzzle surged in popularity all over the country *(1, 2)*.

The following Sudoku puzzle deals with the names and generic structures of organic functional groups found in organic molecules. They do not deal directly with numbers as

	R-COOH					$R\text{-}CONH_2$	$R\text{-}NH_2$	R-CO-R′
$R\text{-}NH_2$	R-Cl	R-CO-R′	R-OH			R-O-R′		
R-O-R′					R-COO-R′		R-Cl	R-OH
R-CO-R′								
R-COO-R′	R-OH		R-O-R′	$R\text{-}NH_2$	R-CO-R′		R-COOH	$R\text{-}CONH_2$
								R-O-R′
$R\text{-}CONH_2$	R-CO-R′		R-COOH					R-Cl
		$R\text{-}NH_2$			R-Cl	R-OH	$R\text{-}CONH_2$	R-COO-R′
R-Cl	R-COO-R′	R-CHO					R-O-R′	

Organic Molecules

Functional Groups

Lipids:
fats, oils, waxes, steroids,
plant natural products (terpenes)

Fats produce 9 to 10 Calories per gram; **More than twice the energy of sugars or proteins, which produce 4 to 5 Calories.**

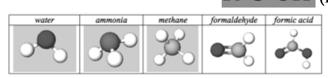
Lipids: Fats & Oils

Lipids are natural plant & animal products more soluble in non-polar solvents like gasoline than in water.

Lipids

Common Functional Groups

Name	General Formula
Alcohols	R–OH (R is very large, note: glycerol is not a lipid)
Ethers	R–O–R′
Amines	$R\text{–}NH_2$
Carboxylic Acids	R-C(=O)-OH (R is very large)



Lipids

Common Functional Groups

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

Lipid Wordsearch

Terry L. Helser
Department of Chemistry, SUNY College at Oneonta, Oneonta, NY 13820-4015; helsertl@oneonta.edu

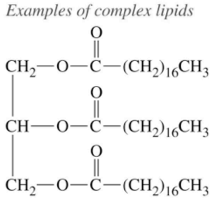
This puzzle contains 37 names, terms, prefixes and acronyms that describe lipids. They may be in any linear direction. Find and highlight these terms in the matrix below. "TRIACYLGLYCEROL" is already done for you. Then, correctly transfer them to the blanks in the description below the matrix. Use the letters remaining in the matrix to complete the sentence describing these molecules. Your success will be rewarded. The answers to the Lipid Wordsearch are found below. Good hunting!

```
N F A T T Y L A I T N E S S E S L
I P O R E T S E A C I D P T T D A
D A C Y L F A T X T I H A S A I N
N O L Y T E C A I P I N S N E P O
A S T P H E W E I N E B F A L I L
L T R I A C Y L G L Y C E R O L I
G E S U E L O O O X I D A T I O N
A R T O L H M N L S T E A R A T E
T O E L P Y I I F M O S A I C I F
S L R S E L P L T Y F I N O P A S
O P O L Y I U N S A T U R A T E D
R H I E D I L O R E T S E L O H C
P N D S D T E R P E N E R P O S I
```

TRIACYLGLYCEROLs are E____s of P________, S_______, and O_____ with glycerol. S_______ them to make S___. B___ O________ cleaves their ____-C__s into A_ _ _ _ _-_ _ _ _s. The E_ _ _ _ _ _ _ _ _ F_ _ _ _ A___s include _________ and ______N___, which are P___U__________ with 2 or 3 C__ double bonds. They are precursors for P____________ hormones and maintain F_ _ _ _ M_ _ _ _ _ _ membranes as part of P_____________ and S______M_____. Hydrogenating such L_____ makes O___, which can contain T____ double bonds. L______ is a W__. Polymers of I_______ form the T______s and other simple L_____ like the S_____, C___________, and ______D hormones.
Use the remaining 16 letters to fill in the following sentence:
_ _ _ _ _ _ _ _ _ _ _ _ for _ _ _ _ .

Molecular Formula: $C_{57}H_{110}O_6$
Molecular weight: 891 amu; MM= 891 g/mol

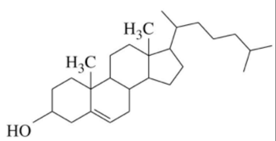
Examples of complex lipids



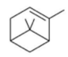
tristearin, a fat

$\Delta_c H^\circ_{solid}$	-35806.7 ± 1.8	kJ/mol

Examples of simple lipids



cholesterol, a steroid

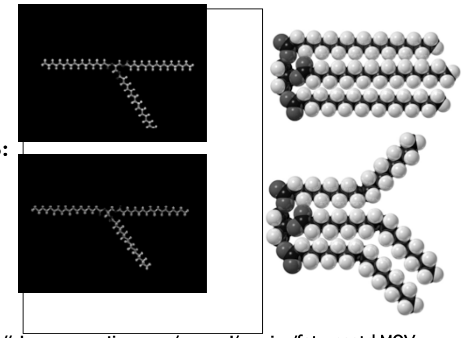


α-pinene, a terpene

C_{10} , C_{15} , C_{20} , etc.

http://chemconnections.org/general/movies/fat-satd.MOV

FATS:



http://chemconnections.org/general/movies/fat-unsatd.MOV

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$R-NH_2$	R-Cl	R-CO-R′	R-OH			R-O-R′		
R-O-R′					R-COO-R′		R-Cl	R-OH
R-CO-R′								
R-COO-R′	R-OH		R-O-R′	$R-NH_2$	R-CO-R′		R-COOH	$R-CONH_2$
								R-O-R′
$R-CONH_2$	R-CO-R′		R-COOH					R-Cl
		$R-NH_2$			R-Cl	R-OH	$R-CONH_2$	R-COO-R′
R-Cl	R-COO-R′	R-CHO					R-O-R′	