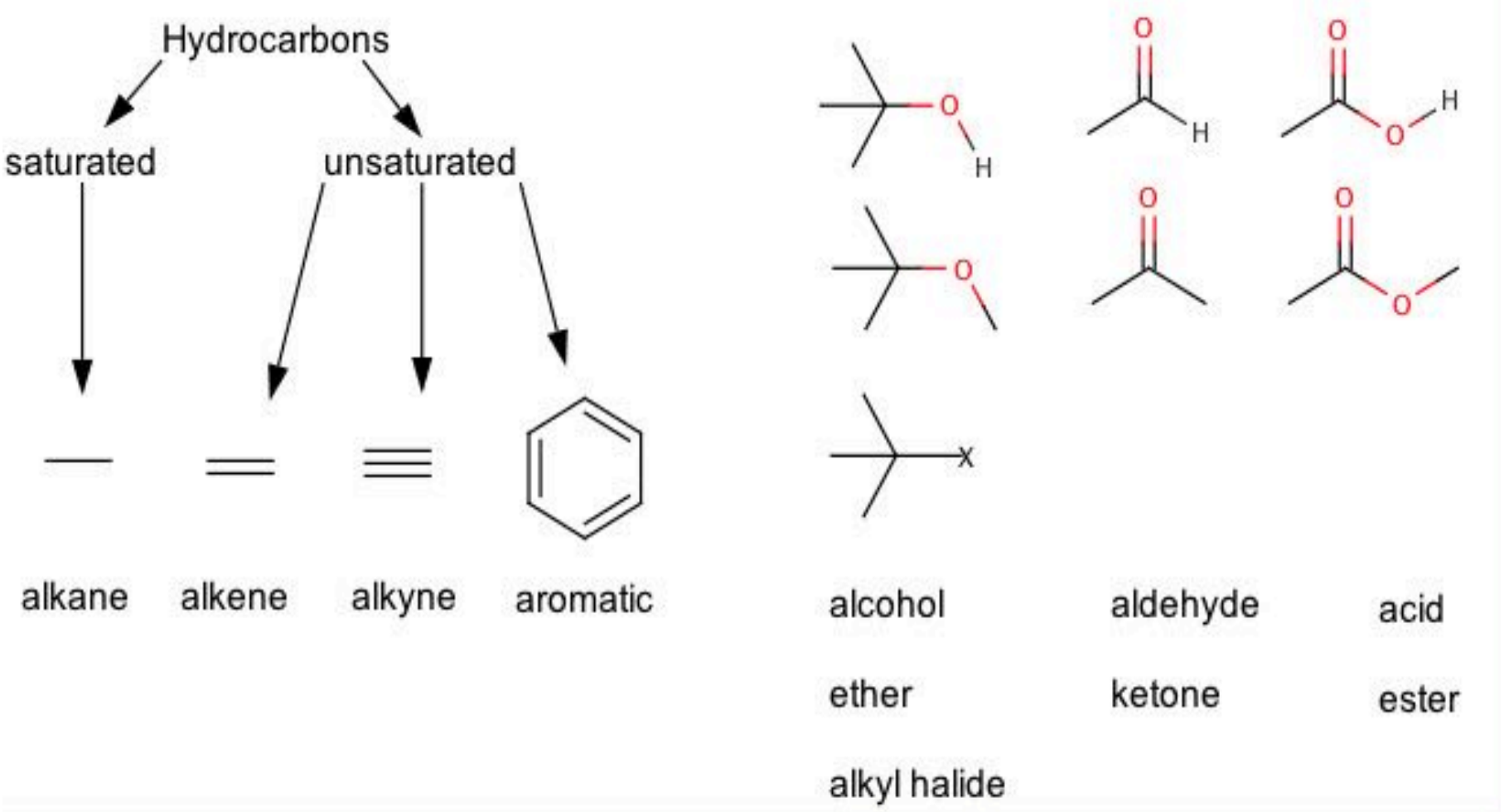
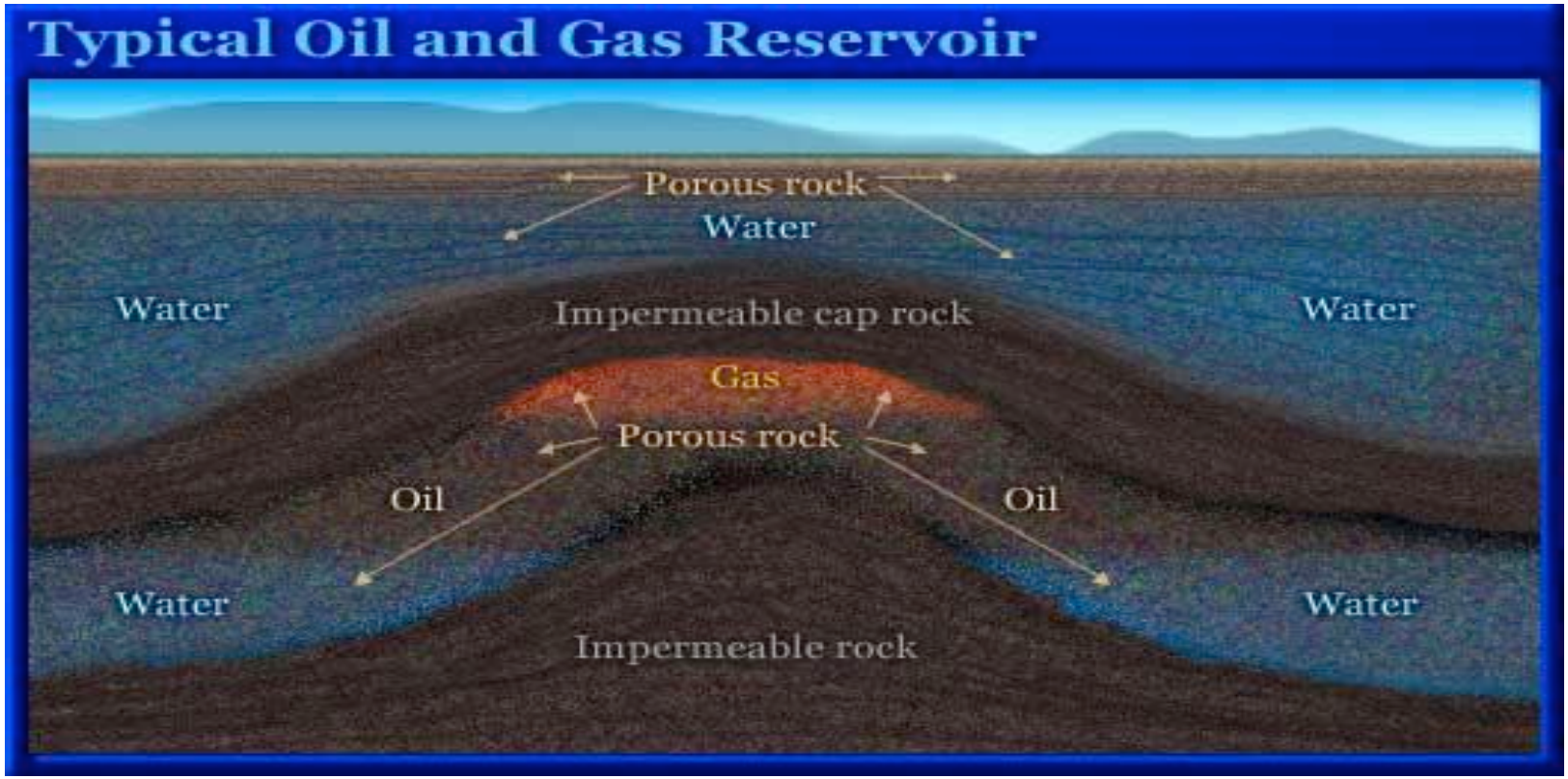
Objective 5

Name alkanes chains and rings – parent and branches.

Organic ***Functional Groups*** Are Small Groups of Atoms With Specific Bonding and Specific Physical and Chemical Properties
What Do These Functional Groups Look Like?





http://www.planetseed.com/node/15250
http://www.oilprimer.com/where-does-oil-come-from.html

Alkanes come from:

a) Plants
b) Petroleum
c) Both
d) None

http://gardeningsolutions.ifas.ufl.edu/mastergardener/outreach/plant_id/flowers_indoor/heart_philodendron.html

Alkanes and Cycloalkanes Contain C and H Only

Hydrocarbons come from Petroleum:
http://www.tutorvista.com/content/chemistry/chemistry-iii/hydrocarbons/petroleum-and-petrochemicals.php

Petroleum components make many useful substances.

Hydrocarbons come from Plants:
waxes
terpenes

CEN, 12/17/07, p. 11 Microorganisms can help squeeze methane out of oil fields

The same microbes that degrade oil could allow oil companies to extract difficult-to-recover energy from oil fields and oil sands through existing infrastructures, according to a new study (Nature, DOI: 10.1038/nature06484.)

Biodegradation:

alkanes in oil ---water---> CH_3COO^- + H_2

CH_3COO^- ---> CO_2 + H_2

CO_2 + H_2 -----> CH_4.

Physical Properties:

Hydrocarbons Are Insoluble in water. *Why?*

Branched Alkanes have lower b.p. and m.p. than straight alkanes.

As # of branches ↑ --> b.p. and m.p. ↓

(branched alkanes do not pack as close together as straight alkanes)

Chemical Properties - Reactivity:

Hydrocarbons are used as ***Fuels*** (combustion reaction)

ΔH of combustion ↑ as # of C ↑ (per mole)

Octane rating: http://en.wikipedia.org/wiki/Octane_rating

Octane rating is not related to heat of combustion.

In general,

Alkanes (C-C and C-H bonds) ***are unreactive*** (polar reactions).

Alkenes, Alkynes (π bonds) are more reactive.

Unless **light** (**radical** reaction) is involved - activates C-H bond

$$R\text{-}H + Cl_2 \xrightarrow{h\upsilon} R\text{-}Cl + HCl$$ (substitution reaction)

Alkanes and Cycloalkanes Contain C and H Only

Saturated Hydrocarbons = 4 single bonds to C (*saturated* w/ H)

- Alkane Chains
- Cycloalkane Rings

Bigger Hydrocarbons (> C_3) Have Isomers:
Isomers are Straight or Branched. *Is an alkane chain really straight?*

Carbon atoms in compounds are classified as 1^o, 2^o, or 3^o

- 1^o = C has 1 C bonded to it
- 2^o = C has 2 C bonded to it
- 3^o = C has 3 C bonded to it

Objective: Classify hydrocarbons

Compound A is:

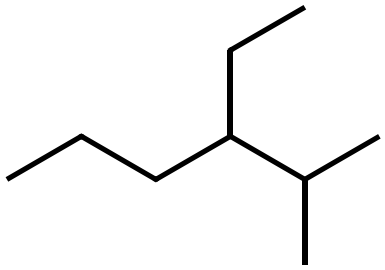
a. straight b. branched

Compound A has _____ carbons.

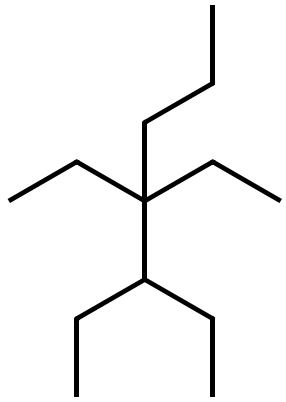
Compound B has _____ 3^o carbons.

Compounds A and B are:

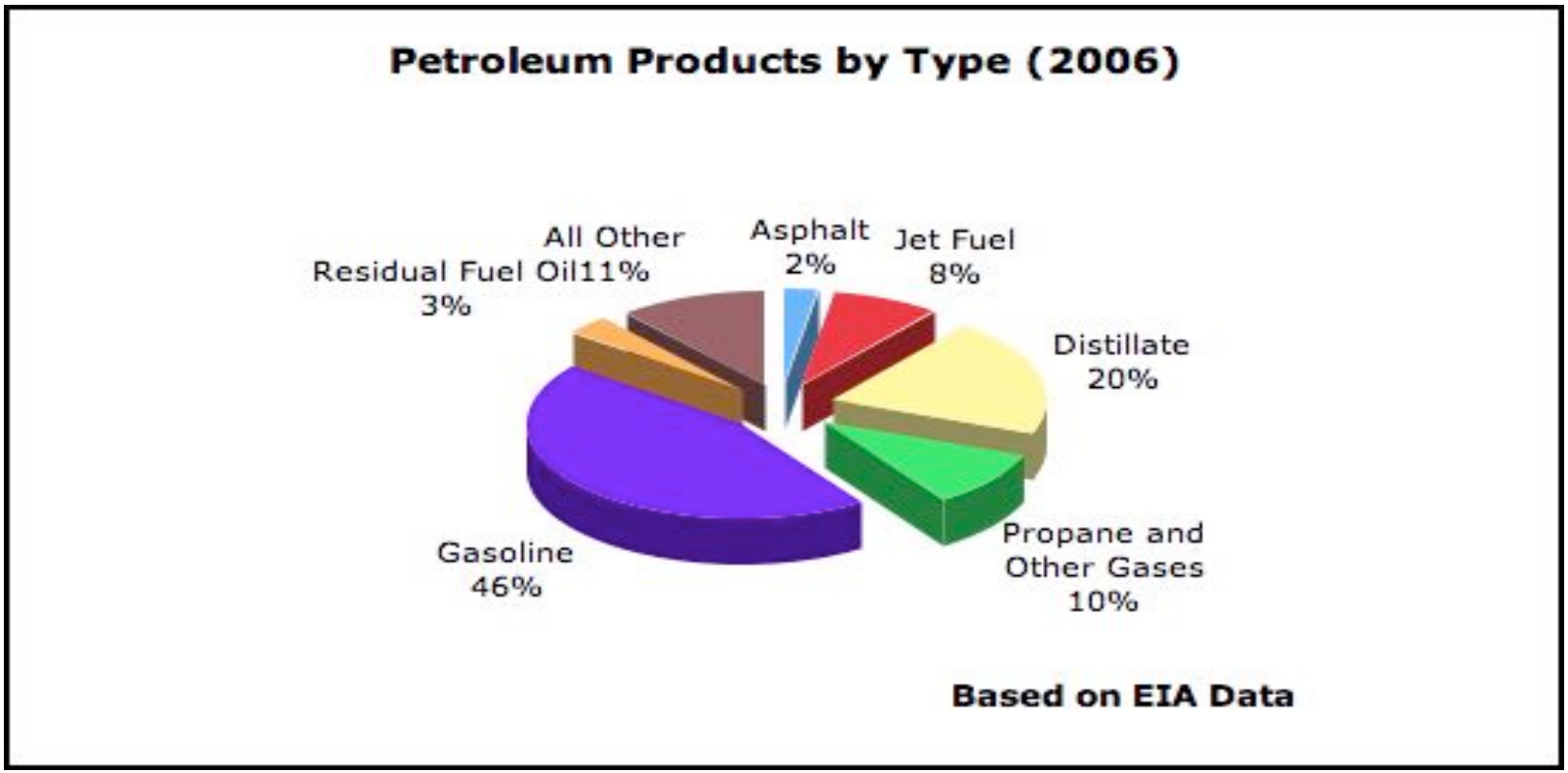
d. same e. isomers f. different



A



B

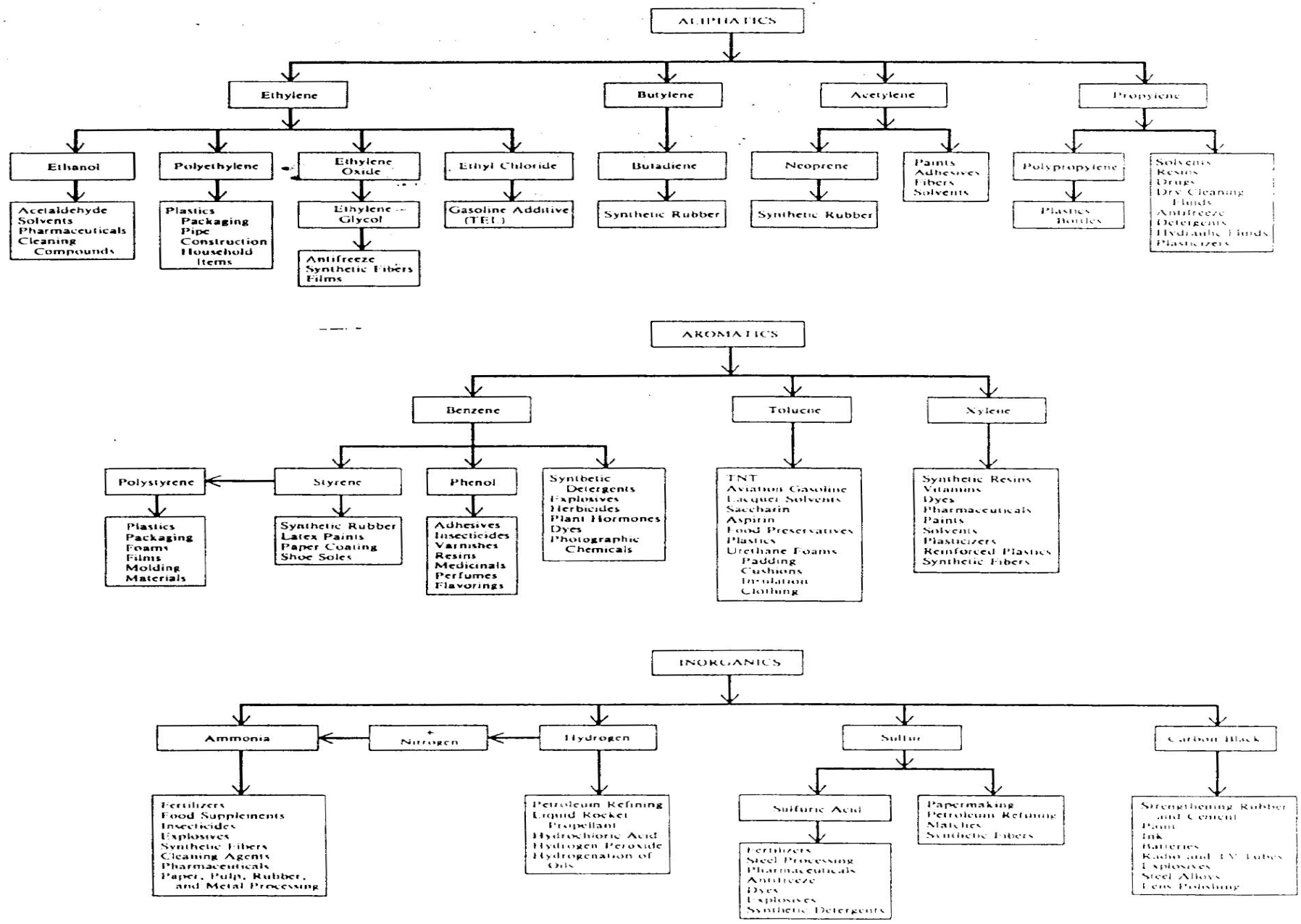


http://www.energybulletin.net/stories/2008-02-24/peak-oil-science-curriculum

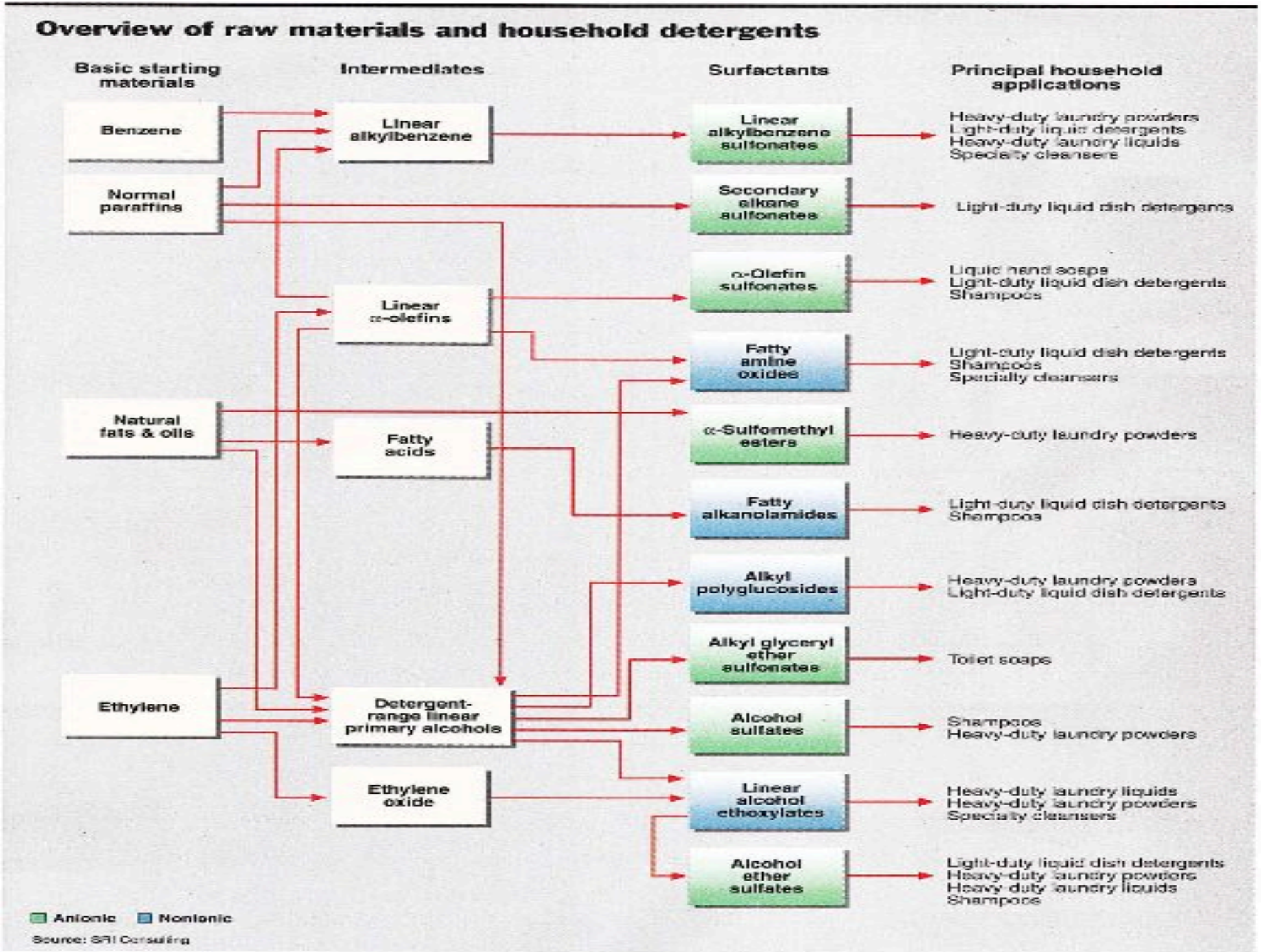
Alkanes are used for or in:

a) Fuel
b) Soaps
c) To make other organic compounds
d) All
e) None

Components of Petroleum Make Many Useful Functional Groups

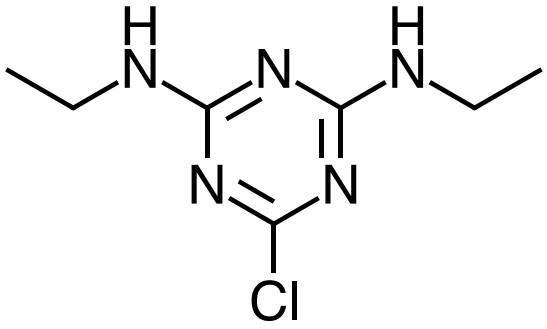


Taken from R. Chang, “Chemistry”, 4th ed., McGraw-Hill

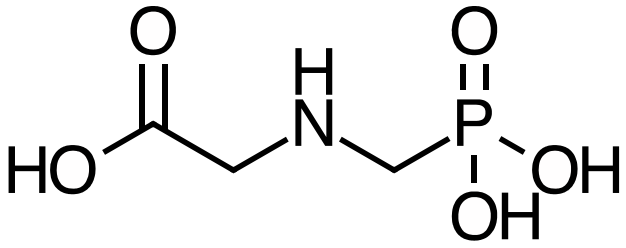


CEN, 2/1/99, "Soaps and Detergents", p. 38

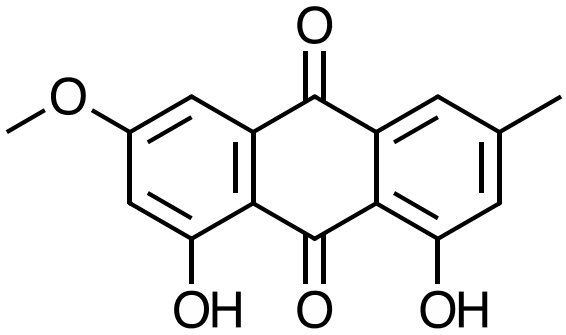
Identify the functional group(s) in each compound



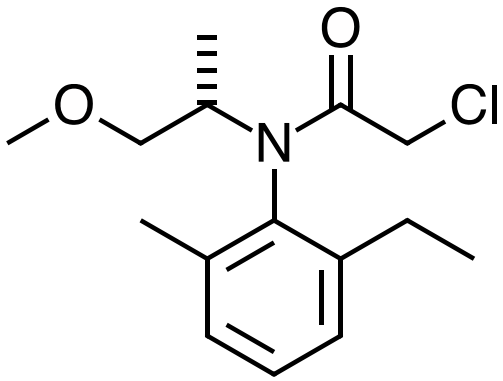
Simazine: herbicide that disrupts photosynthesis but associated with potential health problems



Roundup (Glyphosate): analog of glycine; herbicide that interferes with plant biosynthesis of amino acids. Less toxic than caffeine, aspirin, and table salt



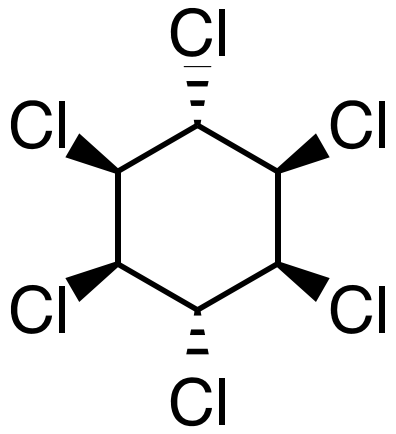
Physcion: fungicide boosts production of proteins and phytochemicals that are active against bacterial and fungal invaders.

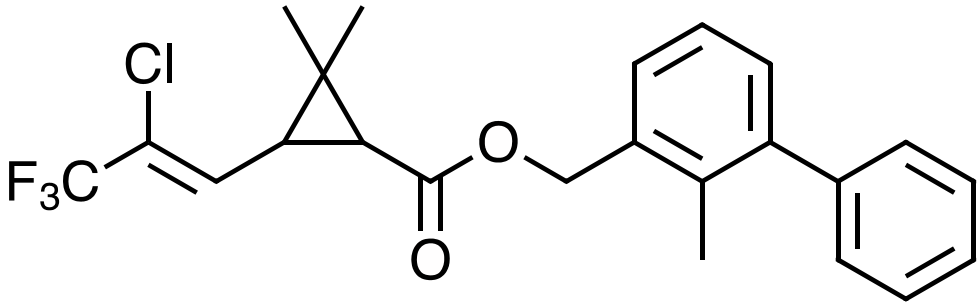


(S)-Metolachlor: herbicide that inhibits plant enzymes.

CEN, 2/16/09, p. 13-20 “Greening the Farm”

Identify the functional group(s) in each compound





Lindane: insecticide (neurotoxin) that kills insects that eats bark on Christmas trees and releases toxin that kills the tree. Persistent in environment. No longer used.

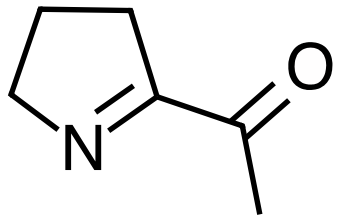
Bifenthrin:insecticide (neurotoxin) that is less toxic and lower application rate than lindane. Synthetic analog of natural insecticidal pyrethrin compounds produced by plants.

CEN, 2/16/09, p. 13-20 “Greening the Farm”

http://cen.acs.org/articles/88/i41/Peanut-Bouquet-Molecules-Identified.html

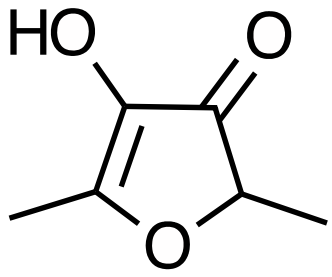
10/11/10, Of the hundreds of volatile compounds in raw peanuts, only 11 contribute to peanut aroma

27 compounds contribute to nutty smell of roasted peanuts.



2-acetyl-1-pyrroline

a common aroma noted in popcorn, crusty wheat bread, and basmati rice



4-hydroxy-2,5-dimethyl-3(2H)-furanone

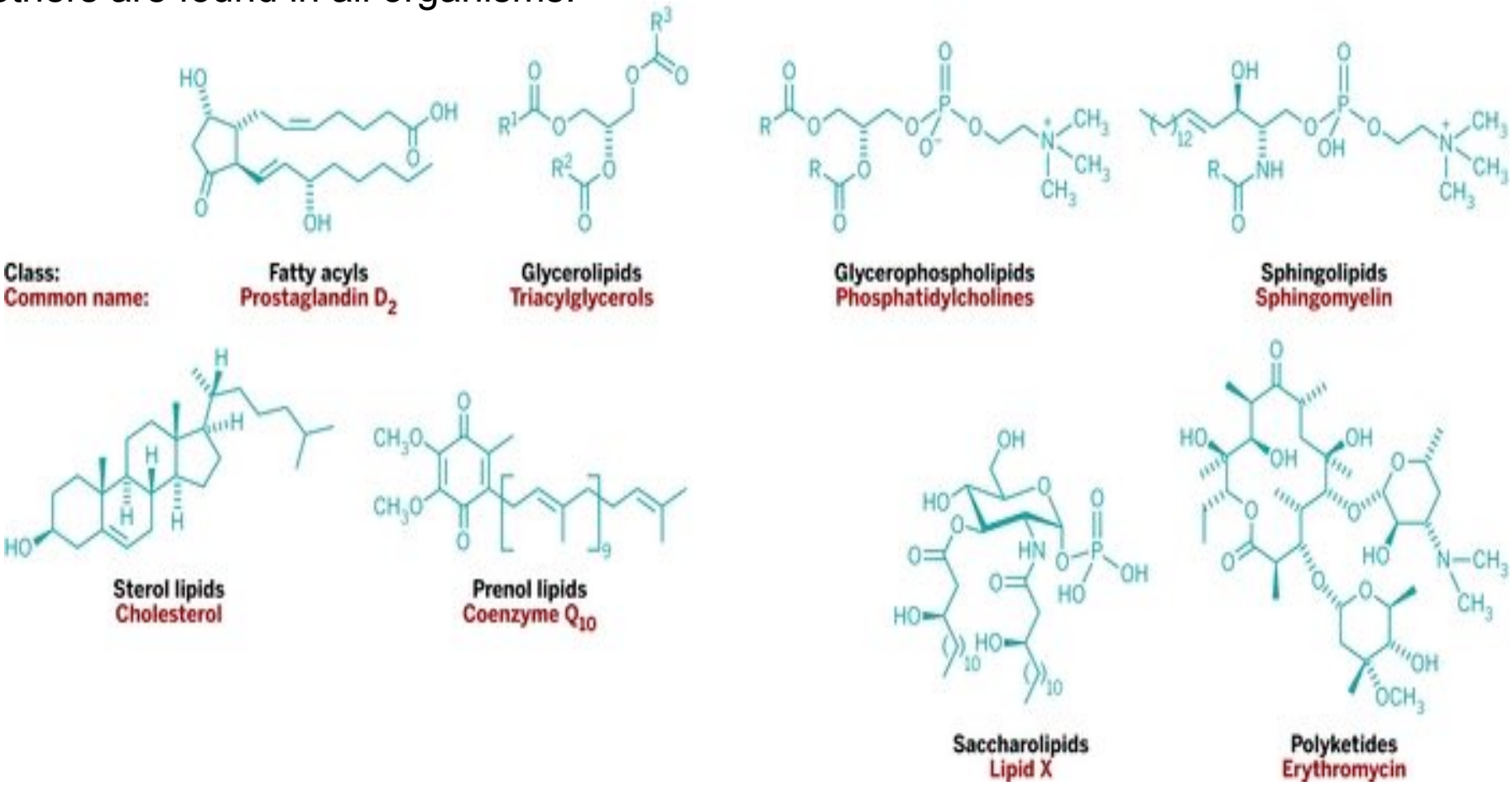
caramel-like fragrance

http://cen.acs.org/articles/89/i41/Lipids-Take-Charge.html

10/10/11, CEN, p. 15 Lipidomics

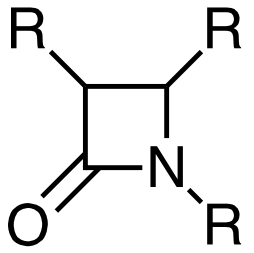
8 Classes of Lipids (LIPID MAPS) based on lipid backbone.

One example from each class is shown here, with the class name and the common name. Saccharolipids and polyketides are found only in plants and bacteria. The others are found in all organisms.

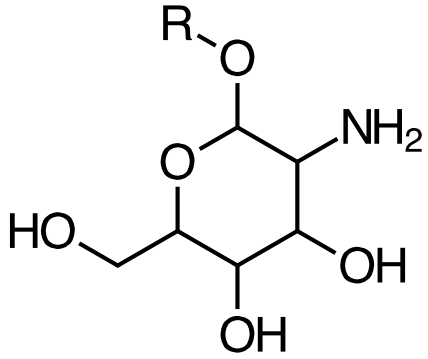


Antibiotics are classified by structure:
(http://www2.wmin.ac.uk/~redwayk/lectures/Antibiotics/Antibiotics.htm#SELECTIVE%20TOXICITY)

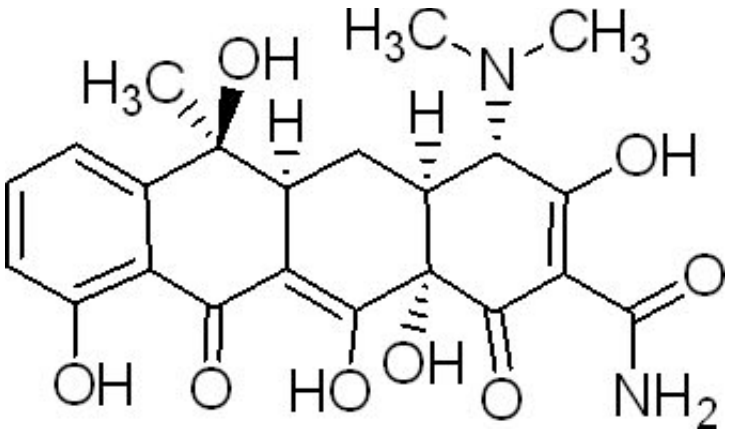
- Beta-lactams
- Aminoglycosides
- Tetracyclines
- Rifamycins
- Macrolides
- Polypeptides
- Chloramphenicols
- Synthetic antibacterials



β-lactam ring



Amino sugar

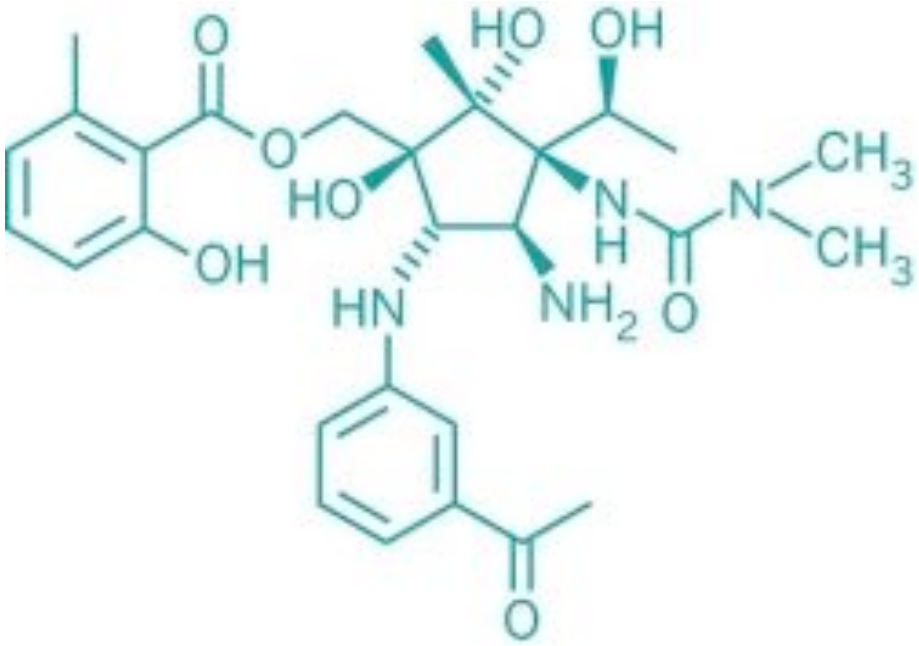


Tetracycline

http://cen.acs.org/articles/91/i15/Rapid-Route-Pactamycin.html

4/15/13, CEN, “Rapid Route To Pactamycin”, p. 8

Pactamycin (from bacterium Streptomyces pactum) has antimicrobial, antitumor, antiviral, and antiprotozoal properties. It disrupts early steps in protein synthesis in bacteria, cancer cells, and mammalian cells.



Pactamycin

Organic Names are Based on the Number of Carbons

# of C	Formula of Chain	Name	Formula of Ring	Name
1	CH_4	Methane		
2	C_2H_6	Ethane		
3	C_3H_8	Propane	C_3H_6	Cyclopropane
4	C_4H_{10}	Butane	C_4H_8	Cyclobutane
5	C_5H_{12}	Pentane	C_5H_{10}	Cyclopentane
6	C_6H_{14}	Hexane	C_6H_{12}	_____
7	C_7H_{16}	_____	C_7H_{14}	_____

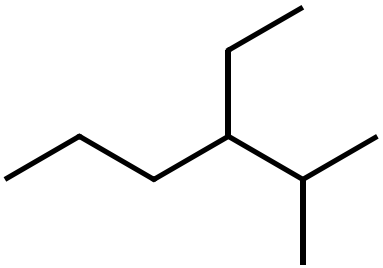
Alkane - 1 H = **Alkyl group** = ***R***. Attach functional group to R

E.g., CH_4 - 1 H = CH_3 CH_3OH

methane methyl group methyl alcohol (methanol)

Objective: Name hydrocarbons

What is the name of this hydrocarbon?

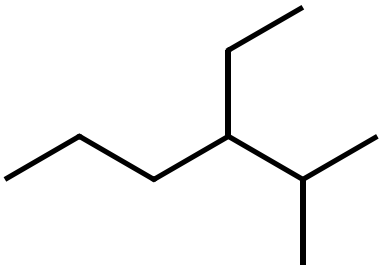


a) 4-ethyl-5-methylhexane
b) 2-methyl-3-ethylhexane
c) 3-ethyl-2-methylhexane

ID parent chain: longest continuous chain = hexane
ID branches: alkyl groups = ethyl and methyl (alphabetical order)
Number the carbons in the parent chain from one end to the other:
use lowest numbers.

Objective: Name hydrocarbons

What is the name of this hydrocarbon?



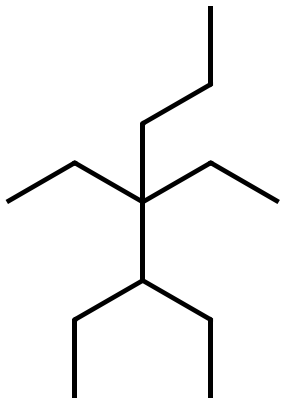
a) 4-ethyl-5-methylhexane
b) 2-methyl-3-ethylhexane
c) 3-ethyl-2-methylhexane

ID parent chain: longest continuous chain = hexane
ID branches: alkyl groups = ethyl and methyl (alphabetical order)
Number the carbons in the parent chain from one end to the other:
use lowest numbers.

Objective: Name hydrocarbons

What is the name of this hydrocarbon?

Enter your choices in your desired sequence. Include numbers on parent chain for branches, commas, and dashes as needed. E.g., 2,3-dimethyl hexane is “2,3-kgc”.



a. butane
b. pentane
c. hexane
d. heptane
e. octane
f. nonane

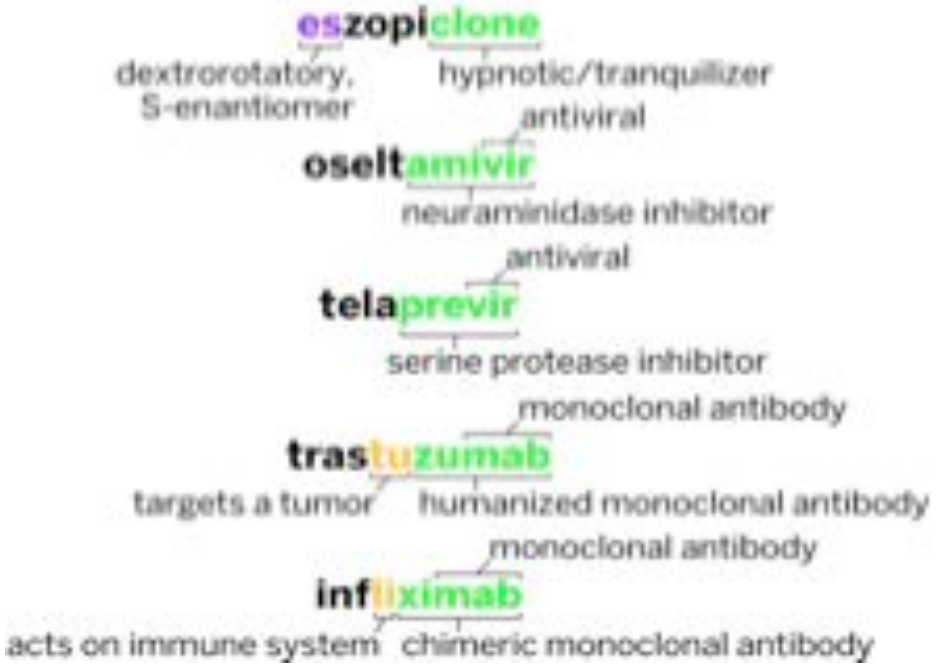
g. methyl
h. ethyl
i. propyl
j. butyl
k. di
l. tri

ID parent chain: longest continuous chain = hexane

ID branches: alkyl groups = ethyl and methyl (alphabetical order)

Number the carbons in the parent chain from one end to the other: use lowest numbers.

How are Drugs named? Where do Drug names come from?
Behind every generic name lies a specific process
http://cen.acs.org/articles/90/i3/Drug-Names-Come.html



http://www.ama-assn.org/resources/doc/usan/stem-list-cumulative.pdf

Chemical Formula gives info about ***# of π Bonds and Rings***
The # of H's relative to C tells us the ***Hydrogen Deficiency Index*** (Degree of Unsaturation)

$$HDI = \frac{(2n+2) - (\#\text{ of H's in formula})}{2}$$

where n = # of C

Formula	# of π Bonds	# of Rings	Example
C_nH_{2n+2}	0	0	Alkane chain = fully saturated
C_nH_{2n}	1	0	Alkene chain
C_nH_{2n}	0	1	Cycloalkane
C_nH_{2n-2}	2	0	Alkyne, _____
C_nH_{2n-2}	0	2	
C_nH_{2n-2}	1	1	Cycloalkene
C_nH_{2n-4}	3	0	
C_nH_{2n-4}	_____	_____	
C_nH_{2n-6}	_____	_____	Benzene

Objective: Relate formula to HDI to help you with structure

Hydrogen Deficiency Index (*Degree of Unsaturation or HDI*) tells you the **number of pi bonds or rings** in a chemical formula.

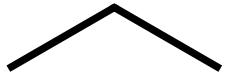
Saturated hydrocarbon chain (alkane): $\mathbf{C_nH_{2n+2}}$

Unsaturated hydrocarbon chain (alkene, alkyne, aromatic): fewer H's than alkane

For hydrocarbon:

HDI = 1/2 (H's in fully saturated - H's in chemical formula)

E.g., C_3H_8 is a saturated hydrocarbon chain.



n = 3

HDI = 1/2 (8 - 8) = 0 so **NO** pi bonds or rings

Objective: Relate formula to HDI to help you with structure

Hydrogen Deficiency Index (*HDI*) tells you the **number of pi bonds or rings** in a chemical formula.

Remember: Saturated hydrocarbon chain (alkane): C_nH_{2n+2}

For hydrocarbon:

HDI = 1/2 (H's in fully saturated - H's in chemical formula)

Index	# of pi bonds	# of rings
0	0	0
1	1 0	0 1
2	2 1 0	0 1 2

What if a compound has X (F, Cl, Br, I), O, or N?

Hydrogen Deficiency Index rules:

- Treat X the same as H (replace X with H)
- Ignore O
- For each N, omit the N and one H

Examples:

C_6H_{12} ==> fully saturated C_6 is C_6H_{14} so Index = 1/2(14-12) = 1

So C_6H_{12} has 1 pi bond or 1 ring.

C_6H_6

C_3H_5Cl ==> same as C_3H_6 so Index = 1/2(8-6) = 1

C_3H_6O

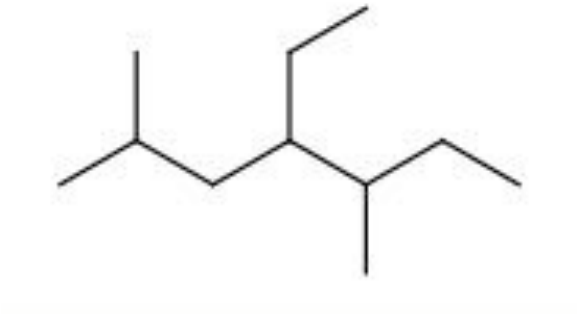
C_2H_7N

Name or draw the structure of the following compounds. Identify the 1°, 2°, and 3° carbons.

a. C_6H_{12}. Does this formula have any isomers? If so, draw an isomer. Name each isomer.

b. 2,3-dimethyl-4-ethylcyclohexane

c.



d. $(CH_3)_2CHCH_2C(CH_3)_2CH_3$