

## Biological Activity

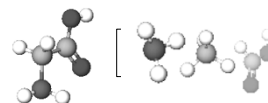
### Molecular Structures Continued Stereospecific interactions of Amino acids / Proteins / Enzymes

Dr. Ron Rusay

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## Amino Acids Legos of Chemical Biology

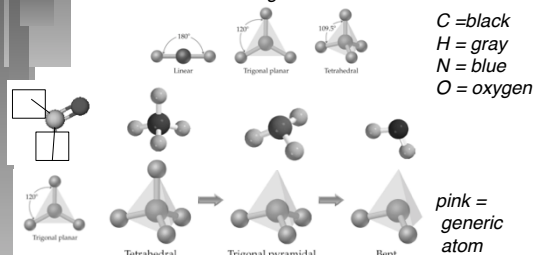
Amino acids contain carbon, hydrogen, oxygen, and nitrogen, which resemble the following shapes & structural components



- 20 different amino acids are encoded by the genetic code, which is archived in DNA.
- Hundreds of amino acids link together to form proteins, which provide the physical structure and chemical machinery for life.
- There are less than 20,000 total proteins produced from humans' entire DNA genome, each coded by a specific gene in DNA's ~3 billion genetic bases.

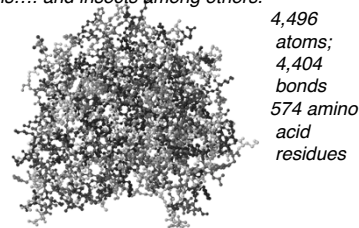
## Lewis Structures → Molecular Shapes Molecular Models for C, H, N, O

- ▶ Fundamental repeating shapes found in every biological molecule



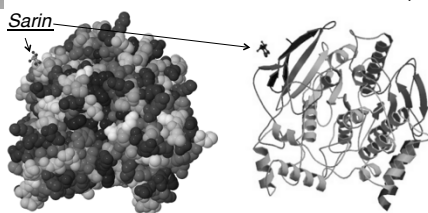
## Proteins: Indispensable Biopolymers Acetylcholinesterase (ACE)

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.



## Proteins & Small Molecules Acetylcholinesterase

Two images with Sarin, a potent nerve agent, which inhibits acetylcholinesterase, and causes convulsions and death if not antidoted with atropine.




## Proteins & Small Molecules Acetylcholinesterase



The ACE enzyme has a receptor, a site in the molecule defined by the 3 amino acids in the image on the right. It binds acetylcholine, which then hydrolyzes. Sarin out competes acetylcholine, binds, and the enzyme cannot work.

## Proteins & Small Molecules

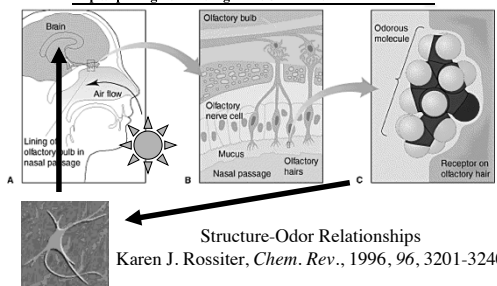
### Acetylcholinesterase



### Detecting molecules we cannot see: the Sense of Smell

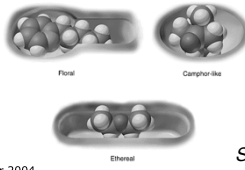
#### Models & Interactions

<http://ep.lnl.gov/msds/orgchem/Chem226/smell-links.html>



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

### Historical view of a few smell receptors.



**Vanillin (Smell)**  
Sensitivity  $\sim 1 \times 10^{-5}$  mol / L<sub>air</sub>

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"

### QUESTION

#### Receptor Sensitivity

If 1.0 gram of vanillin was placed in an open container at center court in the Oakland Coliseum and dispersed, it might be possible to detect it sitting in a seat in the top row.

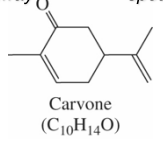
**Vanillin (C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>)**  
Smell detection limit  
 $\sim 1.0 \times 10^{-5}$  mol / Liter<sub>air</sub>

How many grams of vanillin would there be per Liter<sub>air</sub> assuming that vanillin's concentration was at its detection limit?

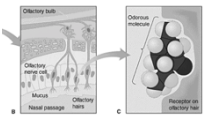
A) 0.015 g  
B) 1.5 mg  
C) 3.0 mg  
D) 0.030 mg

**S-(+)-d-carvone**  
caraway

**R-(-)-l-carvone**  
spearmint

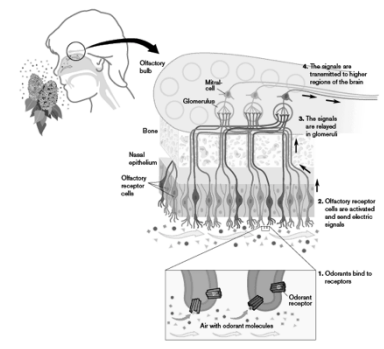


**Carvone**  
(C<sub>10</sub>H<sub>14</sub>O)



They discovered a large gene family, comprised of some 1,000 different genes (three per cent of our genes) that give rise to an equivalent number of olfactory receptor types. These receptors are located on the olfactory receptor cells, which occupy a small area in the upper part of the nasal epithelium and detect the inhaled odorant molecules.

#### Odorant Receptors and the Organization of the Olfactory System

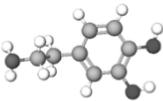


**Opioid Addiction**

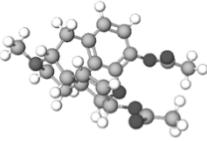
Neurologically active drugs like opioids mimic neurotransmitters that are naturally produced in the body, such as endorphins, which slow breathing, block pain and produce a calming, pleasant, anti-depressing sensation.

However, opiates bind to receptors and flood the nervous system with dopamine, which regulates pleasure among other emotions & functions, producing a level of euphoria that stimulates a craving for more and more, **which can never be satisfied!!!!**

<https://www.sciencedaily.com/releases/2007/10/071014163647.htm>

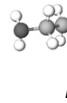


Dopamine



Heroin

However, opiates bind to receptors and flood the nervous system with dopamine, which regulates pleasure among other emotions & functions, producing a level of euphoria that stimulates a craving for more and more, **which can never be satisfied!!!!**



*Dopamine*

*Heroin*

**4N6H: Structure of human delta opioid receptor**


Molar Mass: 52,088.38 g/mol;  
Atoms: 3,481;  
Amino Acid Residues: 414

DOI: 10.2210/pdb-4N6H/pdb  
Classification: SIGNALING PROTEIN  
Organism(s): Escherichia coli, Homo sapiens

**4N6H**

*Trans-membrane*

4N6H



Trans-membrane

[illegible]

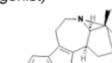
**Agonist:** A substance that initiates a physiological response when combined with a receptor.

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[🔍](#)
[molview.org/?cid=197060](#)


 ibogaine
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### Opioid receptor inhibitor (antagonist)



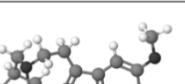
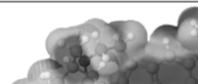
#### Ibogaine

One of several indole alkaloids extracted from Tabernanthe iboga. Ibogaine has a complex pharmacological profile, and interacts with multiple systems of neurotransmission. Ibogaine has anaphrodisiac properties and appears to modulate tolerance to opiates.

|                                |                    |
|--------------------------------|--------------------|
| <b>Formula</b>                 | $C_{19}H_{21}N_2O$ |
| <b>Molecular weight</b>        | 310.441 u          |
| <b>Hydrogen bond donors</b>    | 1                  |
| <b>Hydrogen bond acceptors</b> | 2                  |

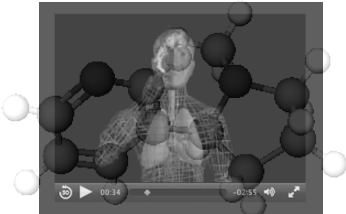
**Percent composition**

|          |                |          |
|----------|----------------|----------|
| <b>C</b> | 12.0107 u x 20 | 77.386 % |
| <b>H</b> | 1.00794 u x 26 | 8.4419 % |
| <b>N</b> | 14.0067 u x 2  | 9.0246 % |
| <b>O</b> | 15.9994 u x 1  | 5.1529 % |

| Percent composition |                               |          |
|---------------------|-------------------------------|----------|
| C                   | $12.0107 \text{ u} \times 20$ | 77.380 % |
| H                   | $1.00794 \text{ u} \times 26$ | 8.4419 % |
| N                   | $14.0067 \text{ u} \times 2$  | 9.0240 % |
| O                   | $15.9994 \text{ u} \times 1$  | 5.1539 % |

<http://chemconnections.org/general/movies/106-nicotine-smoking.mov>

A video player interface showing a man in a plaid shirt smoking a cigarette. Overlaid on the video is a large, semi-transparent ball-and-stick molecular model of a complex organic molecule, likely nicotine. The video player controls at the bottom show a play button, a progress bar at 00:14, a volume icon, and a full-screen icon.