Atomic Resolution Structures: X-ray Diffraction

Proteins must be crystallized in a regular lattice. Crystal quality determines resolution.

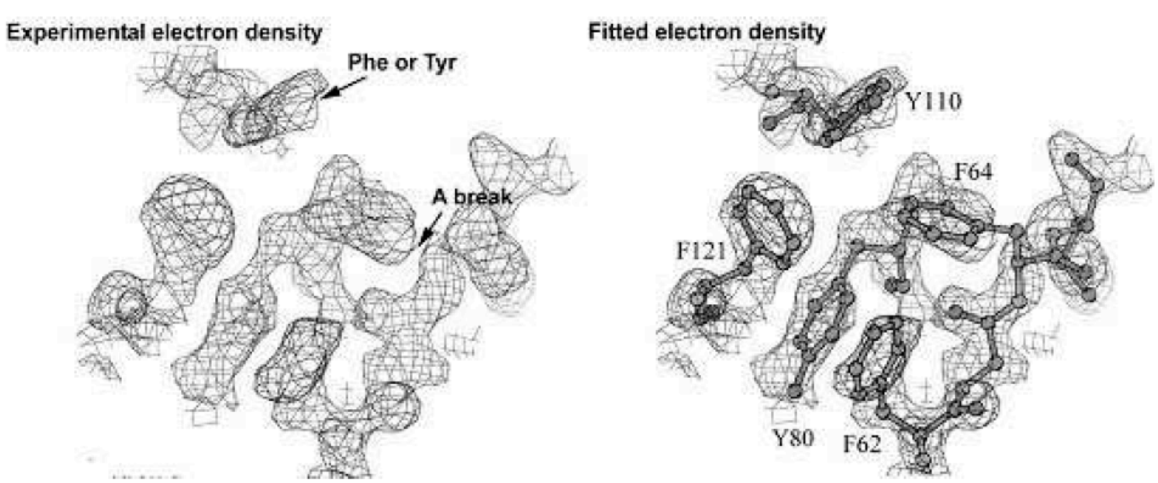
1. No real limitations as to the size of structures.

2. X-rays are scattered by electrons. The amplitude of the wave scattered by an atom is proportional to the number of electrons.

3. The scattered waves recombine. The scattered waves reinforce on another (constructive interference) if they are in phase and cancel each other out (destructive interference) if they are out of phase.

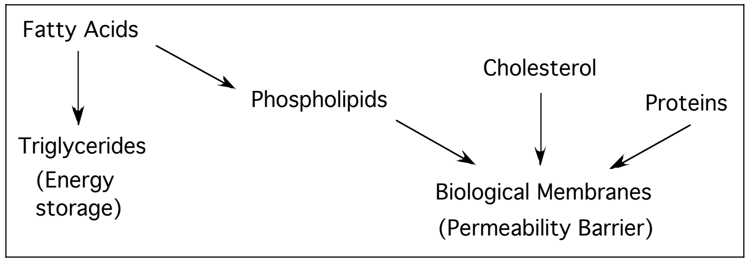
4. The way in which scattered waves recombine depends only on the arrangement of atoms. Therefore, scattered X-rays can be used to determine the position of atoms.

5. Fourier transform of the intensity and phases of the scattered X-rays produces an 'electron density map' or the number of electrons at each point in space in the crystal (□(x,y,z)). The crystallographer must figure out how to place, or "fit", the known primary structure of the protein onto this map (see diagram).



Lecture 22: Lipids

Campbell: Chapter 8.1-8.2

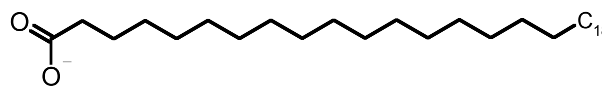


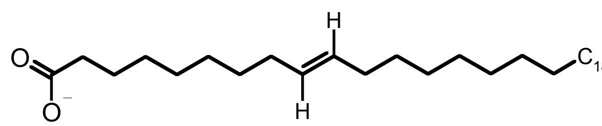
A. Fatty Acids:

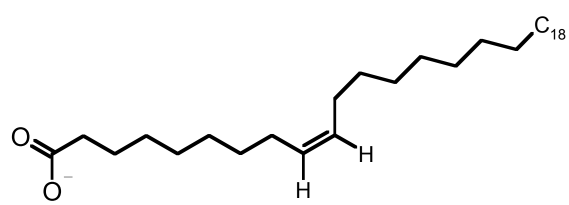
A1. Structure:

A2. Nomenclature for fatty acids:

# Carbons	Name	Melting Temp, C°
12	Laurate	44.2
14	Myristate	53.9
16	Palmitate	63.1
18	**Stearate**	**69.6**
20	Arachidate	76.5
18:1 cΔ9 ($C_9 = C_{10}$)	**Oleate**	**16.0**

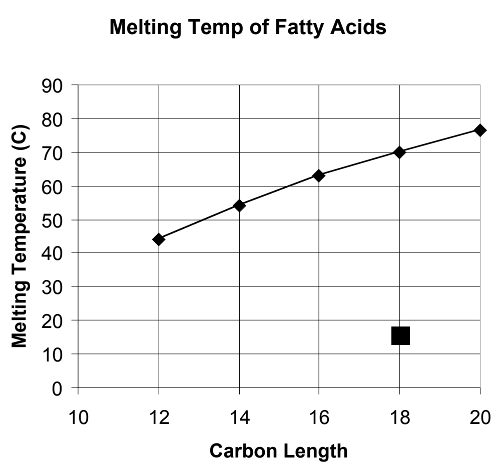






A3. Physical Properties - pure substance

1. The melting temperature depends on the length of the acyl chain due to van der Waals interactions between the chains.
2. This van der Waals interaction is reduced in fatty acids with cis double bonds, causing a *reduction* in the melting temperature (more fluid).



A4. Physical Properties - interaction with water

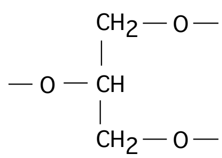
1. Fatty acids form **micelles**, aggregates of fatty acids with a polar (charged) surface and a hydrophobic, waterless, interior. The assembly of micelles is driven by the hydrophobic effect.
2. The non-polar interior

can dissolve hydrophobic compounds (oily 'dirt'). The principal components of soaps are fatty acids and modified fatty acids (*e.g.* SDS) .

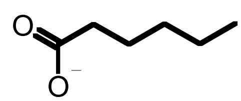
3. *Free* fatty acids are essentially toxic since they can dissolve normal cell membranes in the same way soap would. Fortunately, fatty acids in cells are esterified to glycerol to form triglycerides or phospholipids.

A5. Triacylglycerols (triglycerides) -stores of energy - *not* constituents of biological membranes

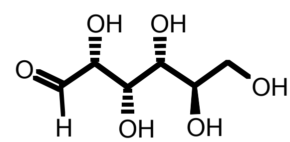
Triacylglycerols are composed of three fatty acyl chains esterified to glycerol.



Triacylglycerols are highly concentrated stores of metabolic energy because they are reduced and anhydrous. They are stored in the form of lipid droplets in adipose cells. Lipids are richer energy sources than sugars because they are less oxidized than carbohydrates.



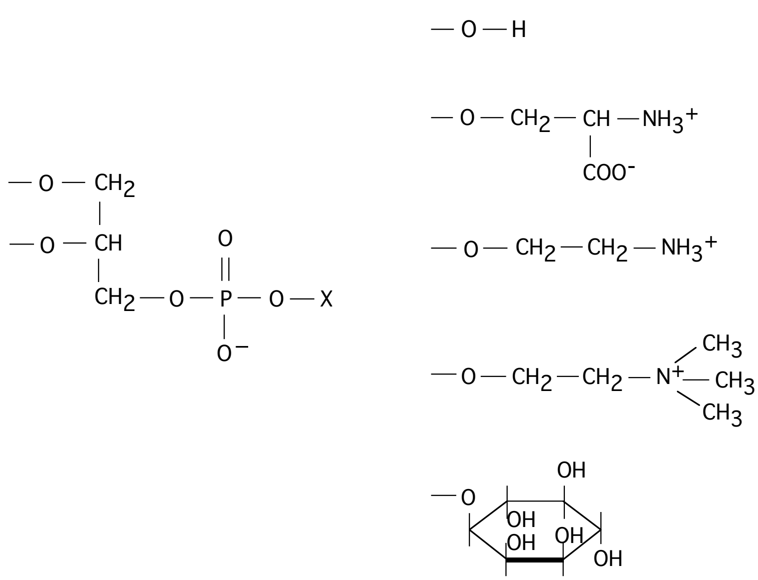
6 carbon fatty acid



6 carbon sugar

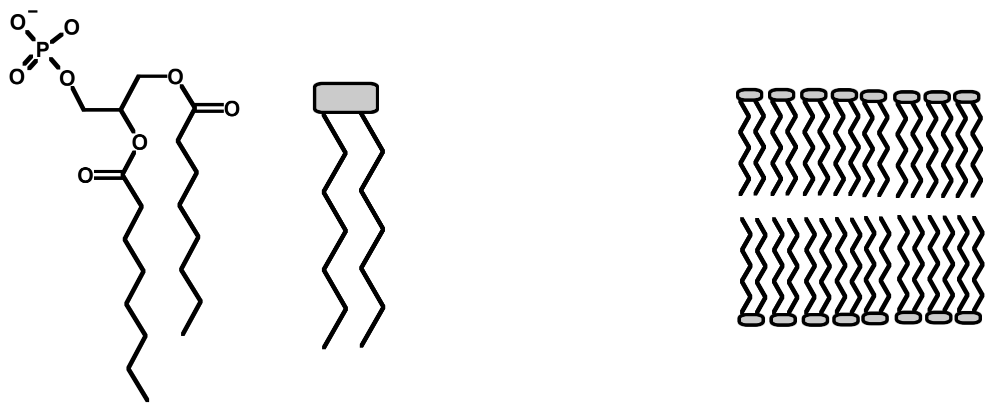
A6. Phospholipids - major constituents of biological membranes

Phospholipids are composed of two fatty acyl chains esterified to glycerol 3-phosphate. In most phospholipids the phosphate group is also esterified to an alcohol. Resulting phospholipids are usually either zwitterionic or have a net negative charge.



Physical Properties

1. Phospholipids self-assemble spontaneously in water to form bilayers (two opposing layers of phospholipids). Bilayers are formed instead of micelles because the cross section of the head group is roughly equal to the cross section of the 2 fatty acid chains.



2. The bilayers form closed, water filled, compartments with a 60-90A° thick wall.
3. Permeability properties:
   - Charged compounds do **<u>not</u>** cross the bilayer.
   - Polar compounds cross infrequently.
   - Non-polar compounds cross readily.