Amino Acids, Polypeptides and Proteins

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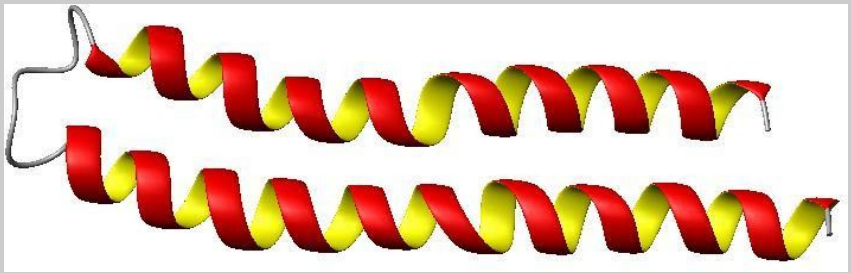
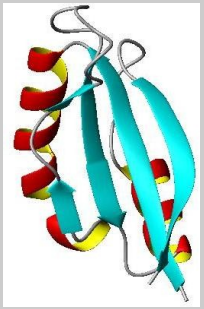
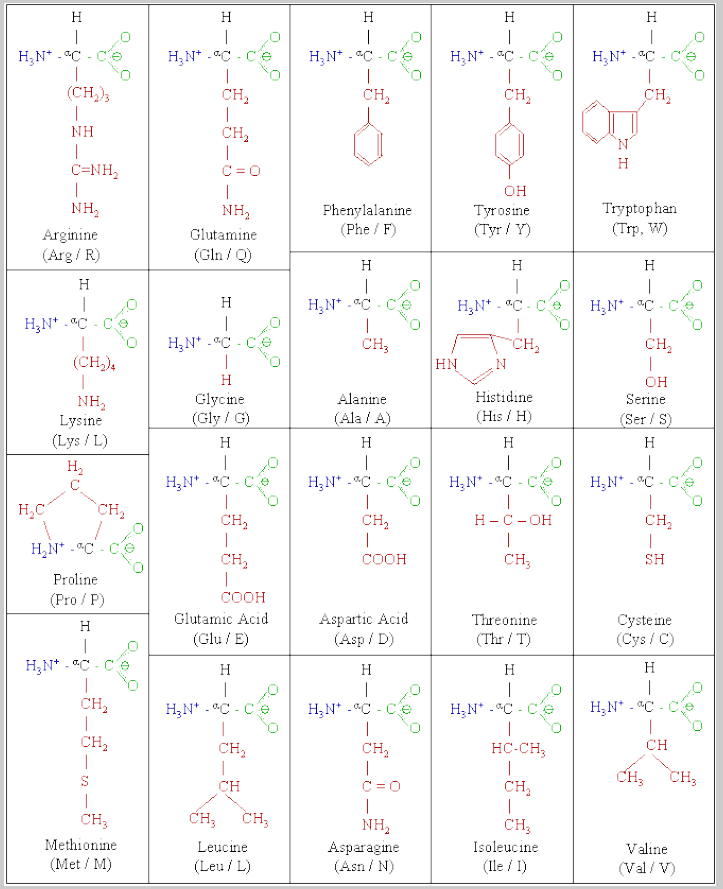
Protein

- Proteins are functional elements of a cell
- Proteins are made of 20 “ amino acid” subunits
- Proteins fold to create a their own characteristic fold (three dimensional shape)

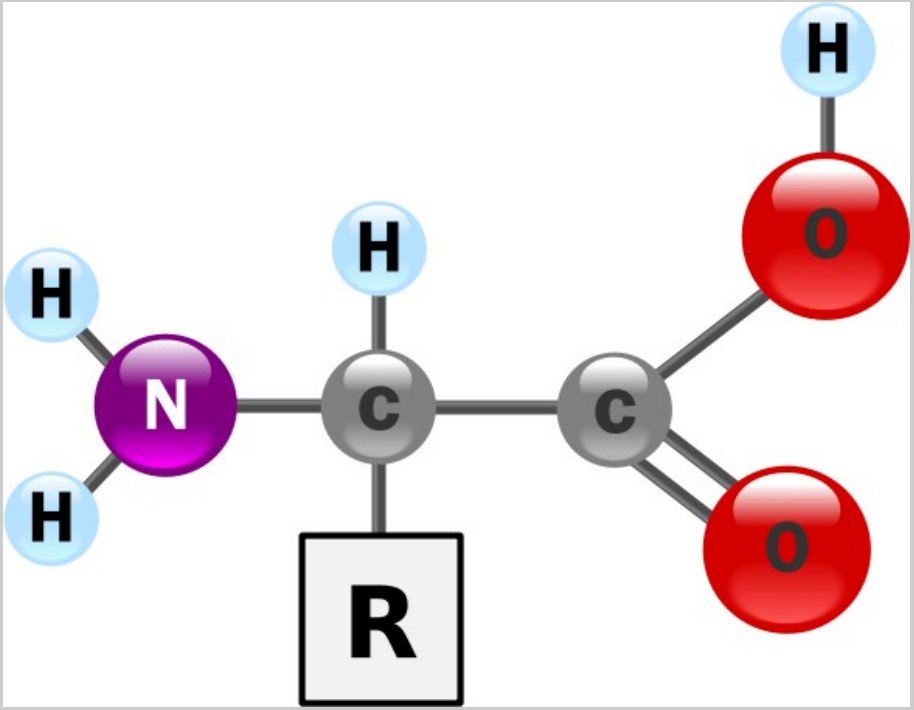






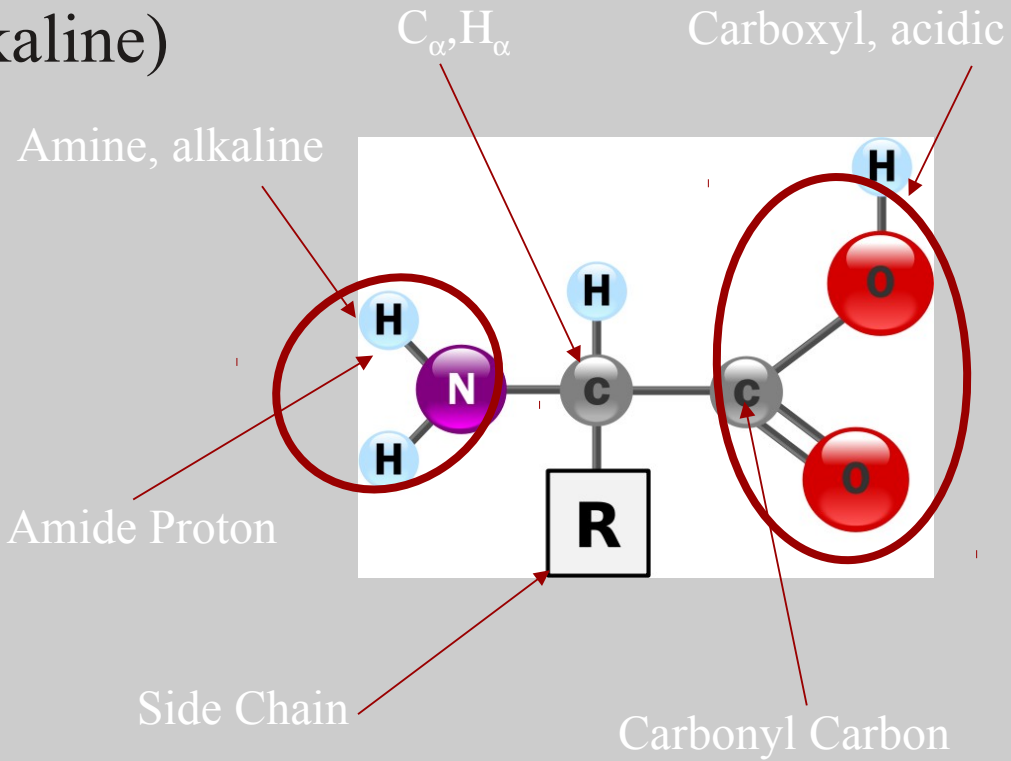
Amino Acids

- 20 amino acids
- General structure of an A.A.
- Differences due to side chain R
- Can be categorized as acidic/alkaline, hydrophobic/hydrophilic or positively/negatively charged



Anatomy of Amino Acids

- Much simpler structure compared to nucleotides
- Side chain R
- Carboxylic group (acidic)
- Amide/amine group (alkaline)
- Zwitterion
- C_α and H_α
- Amide proton
- Carbonyl carbon

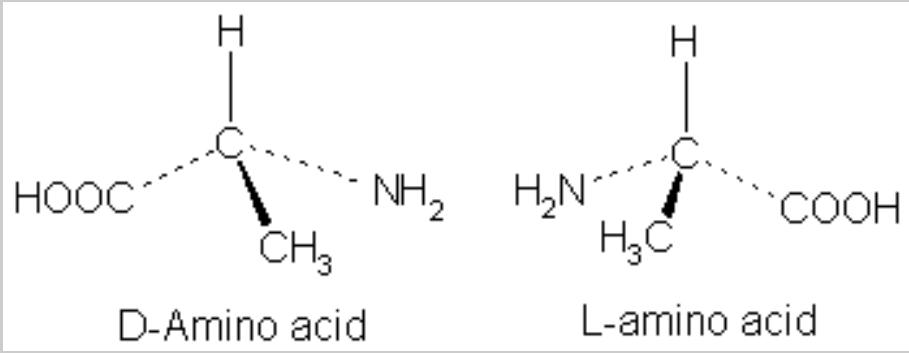


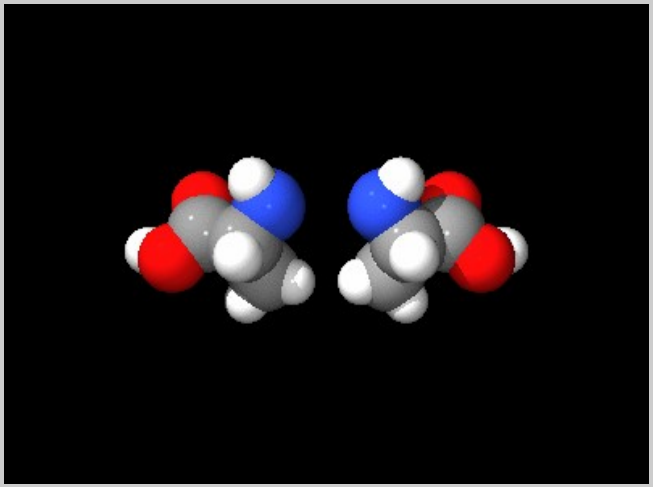
Chemical/Physical Properties of A.A.

- Hydrophobic versus hydrophilic
- Isoelectric point (pI)
- Acidic versus alkaline (basic)
- Mass
- Amino acid full names, three letter and single letter abbreviations
  - Alanine, ALA, A
- Etc.

Stereo Chemistry of Amino Acids

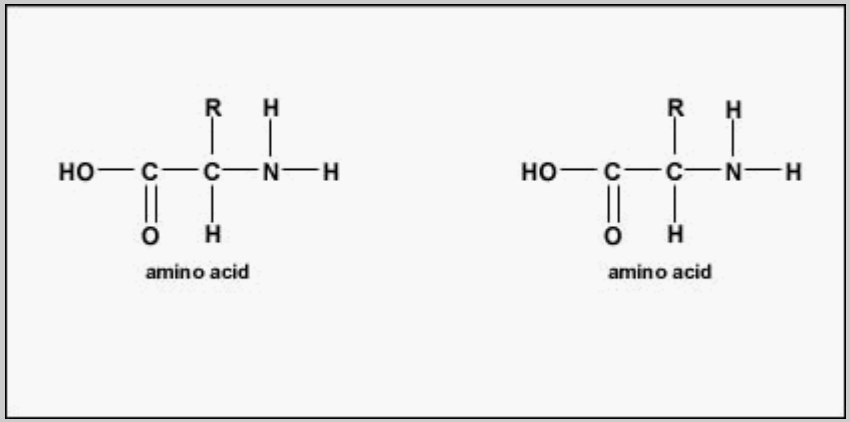
- Amino acids are three dimensional entities
- Carbon forms 4 bonds
- In SP^3 hybridization, these four bonds form a tetrahedron
- Stereoisomer: two identical molecules that can not be superimposed
- D and L are two different enantiomers
- A mixture of equal amounts of both enantiomers is said to be a racemic mixture
- Vast majority of a.a. found in proteins are L a.a.





Peptide (Polymerization of A.A.)

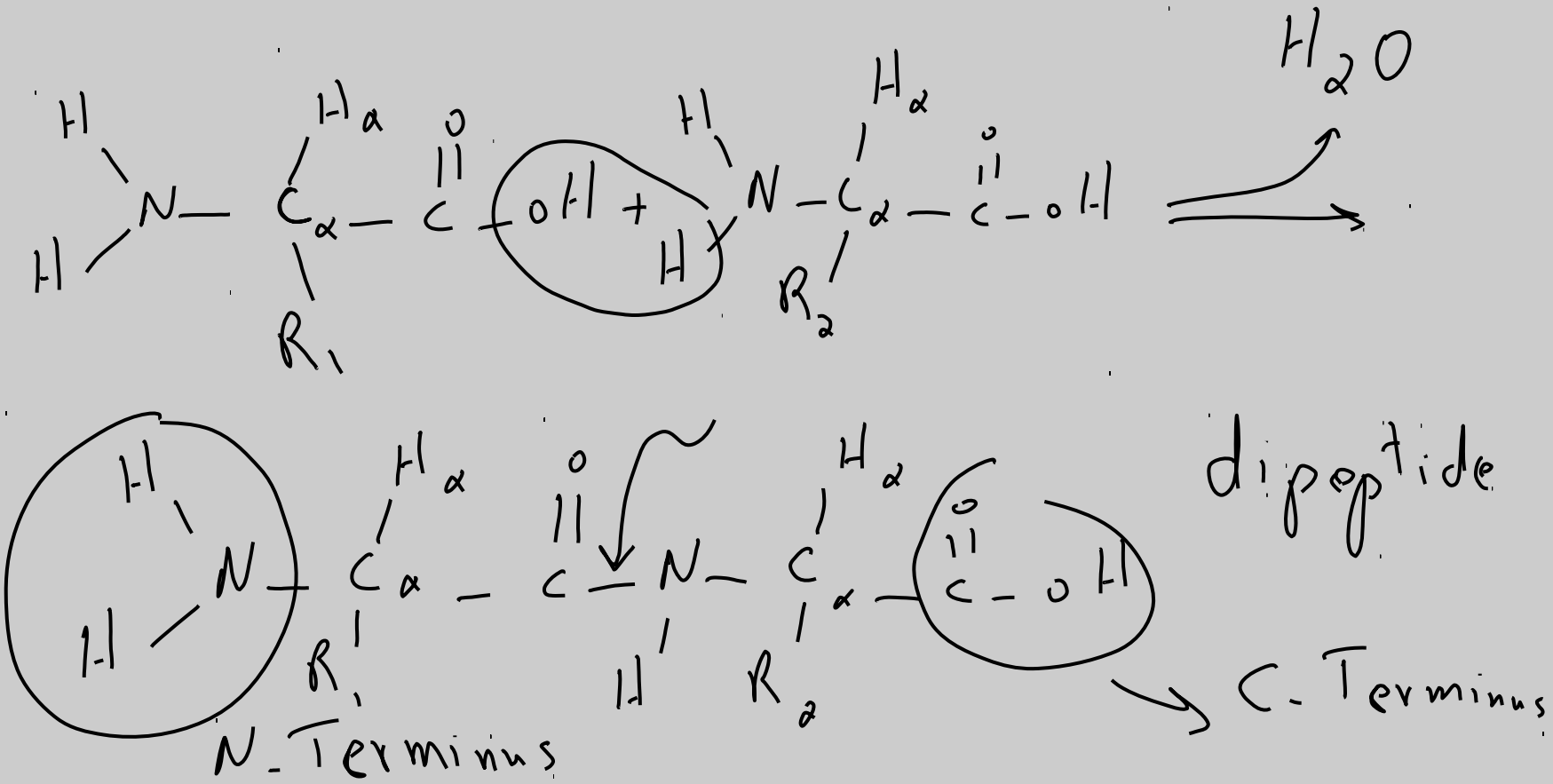
- The family of molecules formed from the linking of various amino acids.
- Two amino acids link through an amide bond or peptide bond.



- Two linked amino acids form a peptide plane (more later).

Polymerization of A.A.

- N-terminus, C-terminus



Polymerization of A.A.

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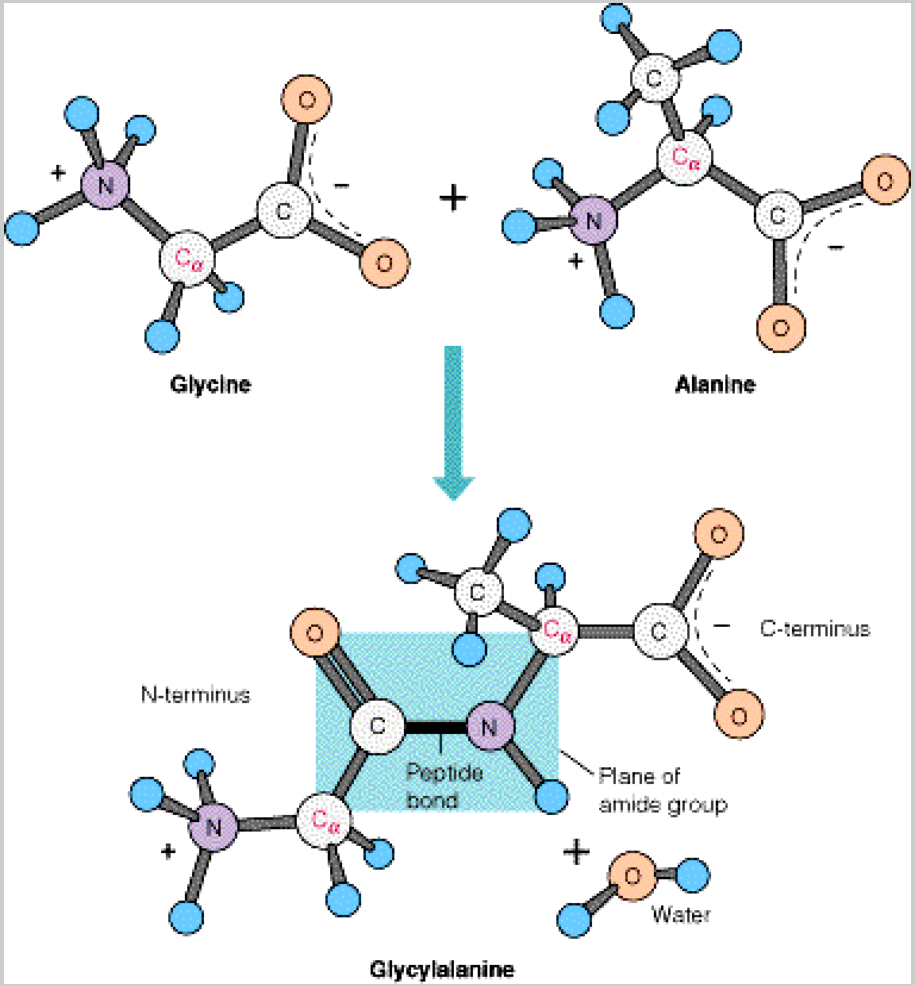
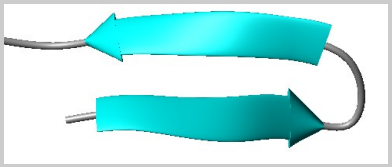


Protein Structure Hierarchy

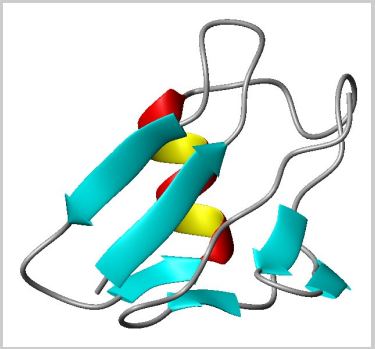
- Primary sequence (1º):
  - linear order of connected amino acids.

    ALA-GLY-LYS-PRO-…
- Secondary Structure (2º):
  - Internal stable segments.

α Helix 

β Strand 

- Tertiary Structure (3º):



Protein Data Bank (PDB)

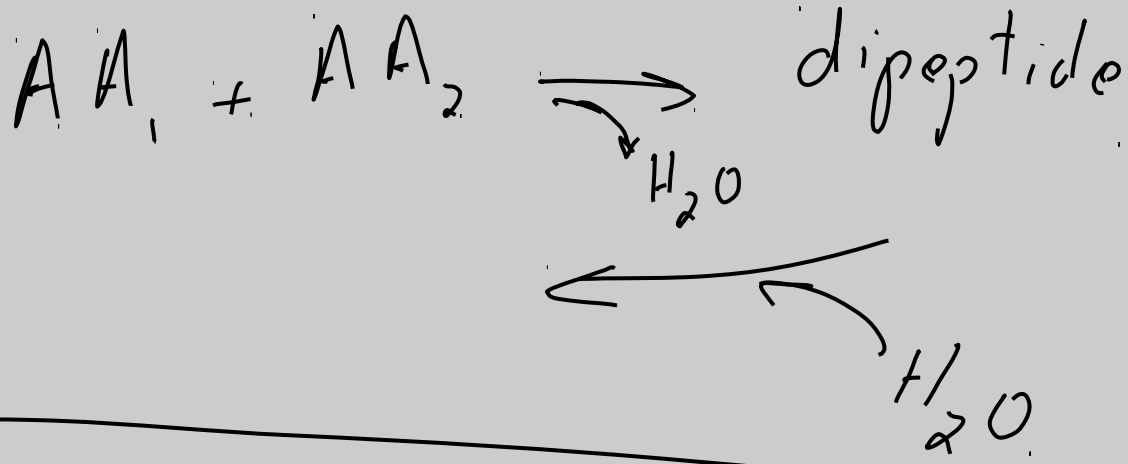
- Most prominent database of structures.
- Contains structures for proteins, DNA, RNA, carbohydrates and other biomolecules.
- Data disseminated in two formats: PDB and mmCIF.
- Become familiar with this database!
  - Learn to download files and use them.
  - Learn search and other various tools on this site.
  - Browse links…

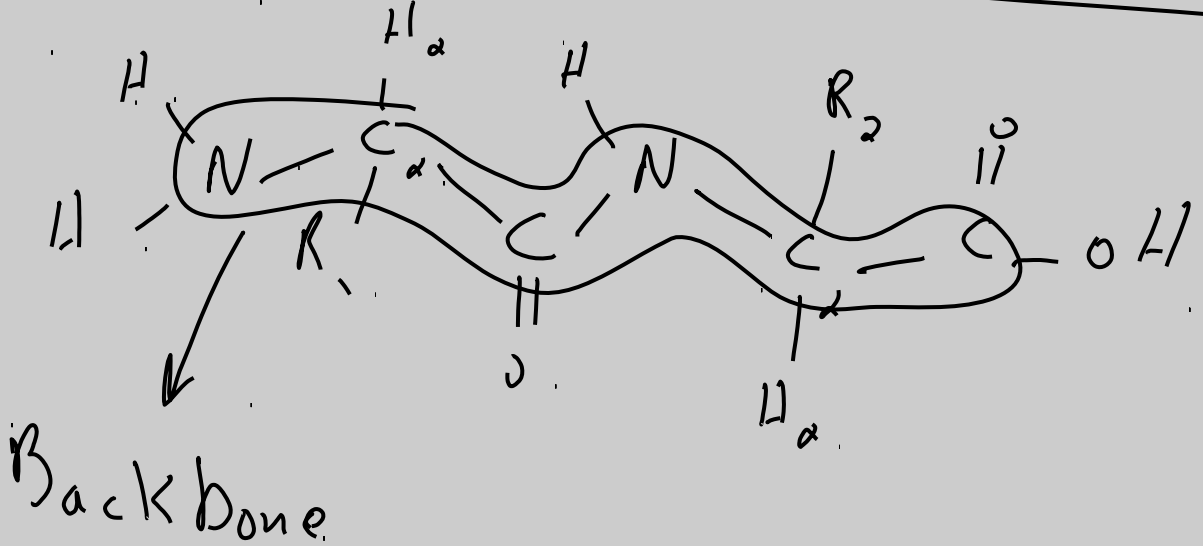
Molecular Visualization Tools

- A number of tools available or different computing environments.
  - Rasmol
  - MolMol
  - PyMol
  - VMD
  - Etc.

Why Protein Structure?

- Proteins provide metabolic and mechanical support for biological organisms.
- Structure gives rise to function.
- Structure is necessary (not sufficient) for function.
- Proteins are of special interest due to their therapeutic potential (why not DNA)?


AA1 + AA2
dipeptide
H2O
H2O


Hα
H
H
R2
O
N
Cα
N
H
R
C
C
C
OH
O
Hα
Backbone