BINF 731

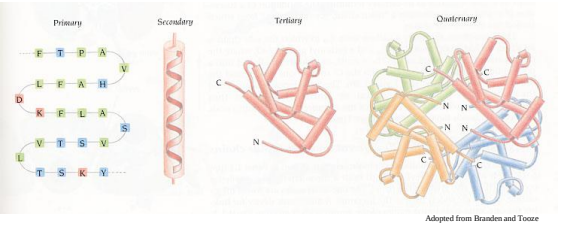
Protein Structure Analysis

http://binf.gmu.edu/vaisman/binf731/

Iosif Vaisman

2023

Protein Structure Hierarchy



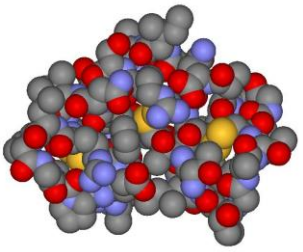
Adopted from Branden and Tooze

- Primary - the sequence of amino acid residues
- Secondary - ordered regions of primary sequence (helices, beta-sheets, turns)
- Tertiary - the three-dimensional fold of a protein subunit
- Quaternary - the arrangement of subunits in oligomers.

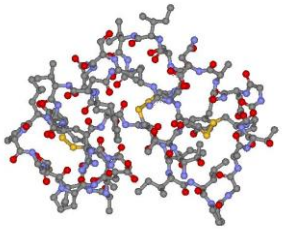
Secondary Structure: Computational Problems

Secondary structure characterization
Secondary structure assignment
Secondary structure prediction
Protein structure classification

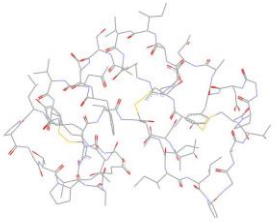
Protein representations



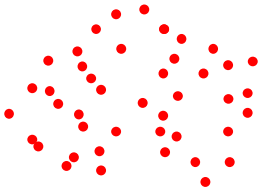
Protein representations



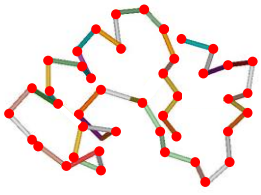
Protein representations



Protein representations

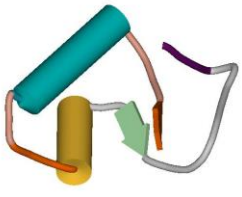


Protein representations

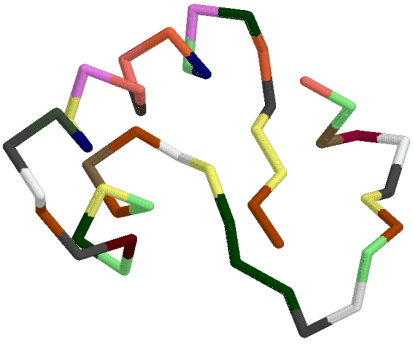


Protein representations

Protein representations

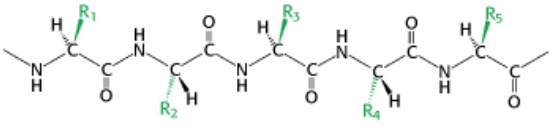


Protein backbone

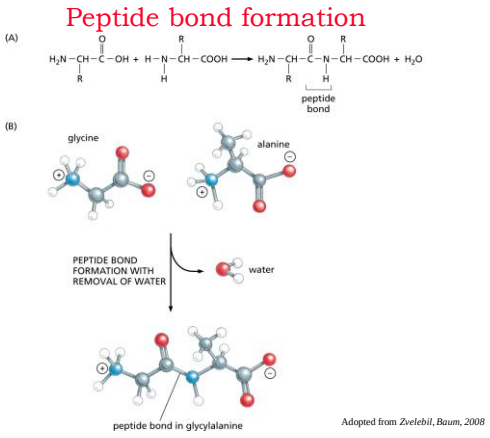


NWVLSTAADMQGVVTDGMASGLDKD

Protein backbone

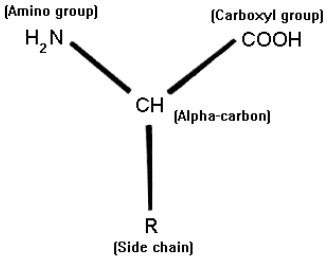


Peptide bond formation

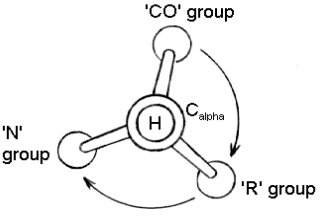


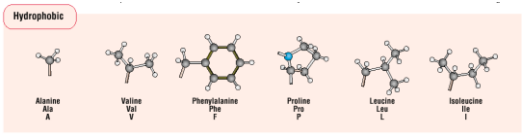
Adopted from *Zvelebil, Baum, 2008*

Amino Acid Residue

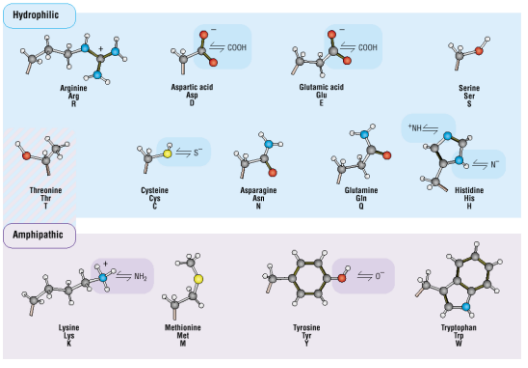


Amino Acid Residue



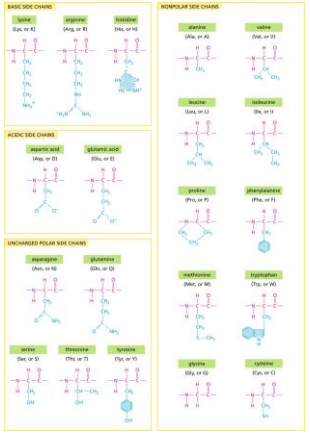


Amino Acids



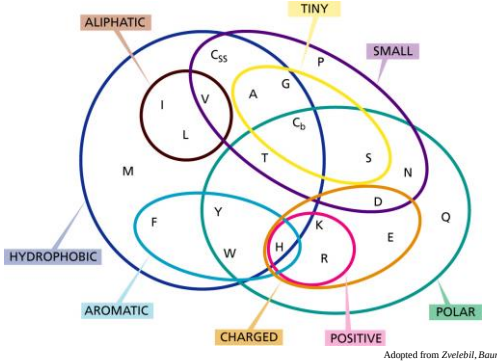
Adopted from: Gregory Petsko and Dagmar Ringe
Protein Structure and Function: From Sequence to Consequence

Amino Acids



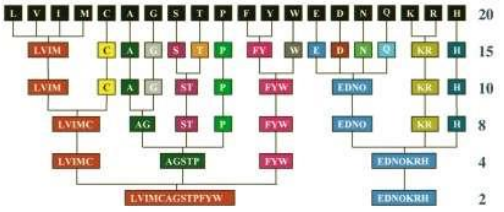
Adopted from *Zvelebil, Baum, 2008*

Amino Acid Residue Clustering



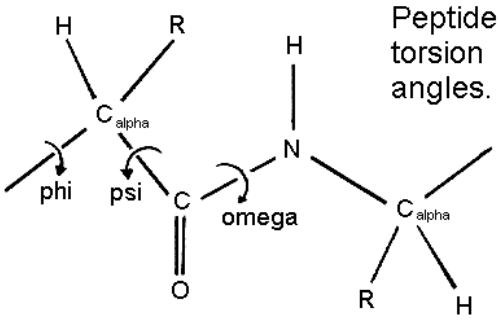
Adopted from *Zvelebil, Baum, 2008*

Amino Acid Residue Clustering

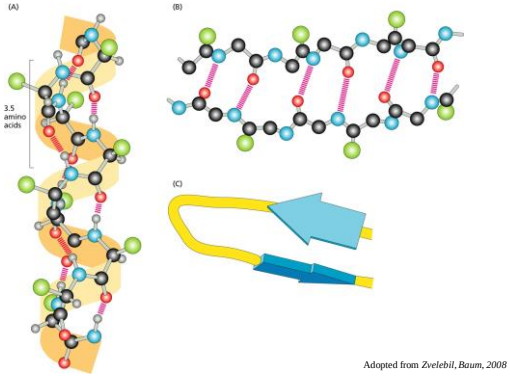


Adopted from: L.R.Murphy et al., 2000

Peptide torsion angles.

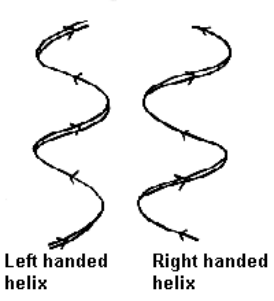


Secondary Structures

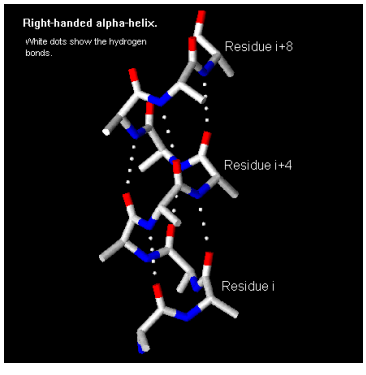


Adopted from *Zvelebil, Baum, 2008*

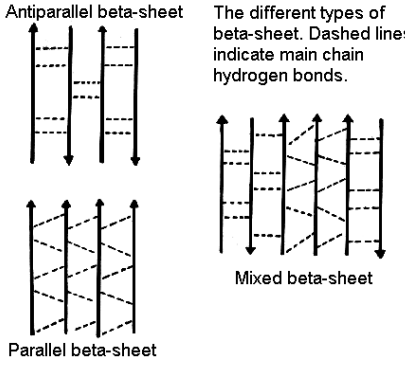
Secondary Structure (Helices)

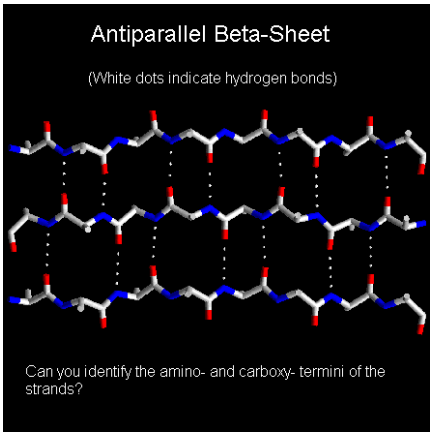


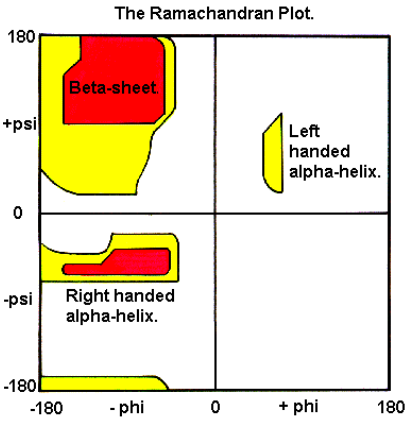
Helix

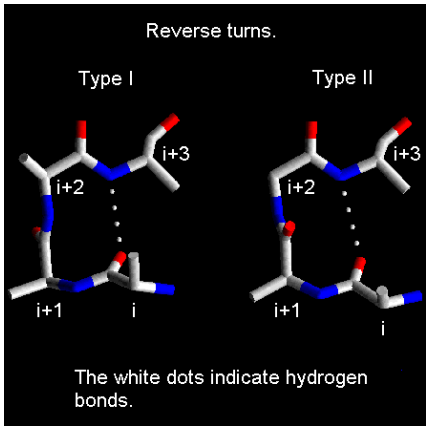


Secondary Structure (Beta-sheets)

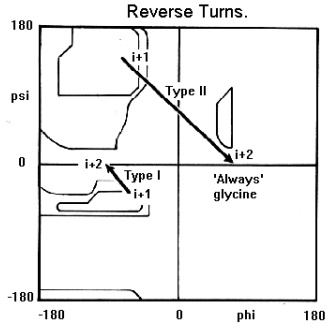


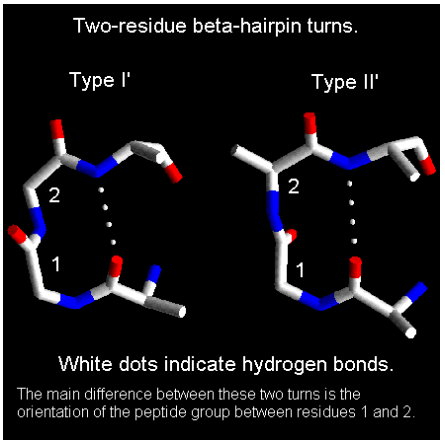




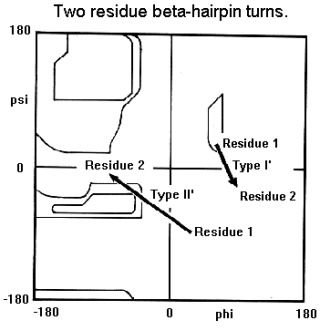


Reverse Turns on a Ramachandran Plot

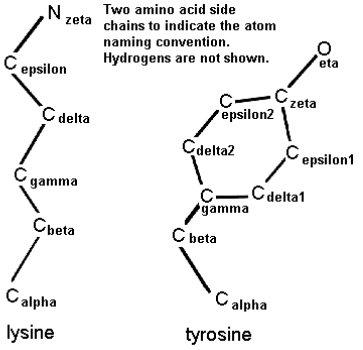




Beta-hairpin Turns on a Ramachandran Plot



Side-Chain Atom Nomenclature



Side-Chain Torsional Angles