

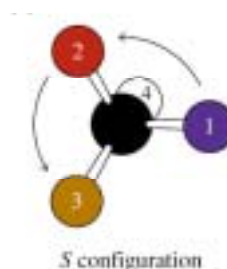
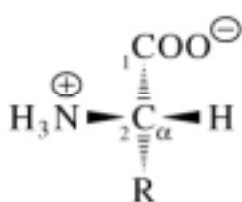
台大生化科技學系 生化實驗  
分子模型建構  
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In this practical, you will learn how to build a peptide model starting from atoms and amino acids. One of the most important issues in biochemistry is the structure-function relationship of proteins. The protein structures are determined experimentally by x-ray crystallography and/or NMR. For those proteins homologous to other structure-determined proteins with over 30% similarity, homology modeling can generally give pretty good model. Protein 3D structures are described by their coordinates". Molecular graphic tools help you to visualize protein structures in computer. SwissPDB Viewer is good software for molecular graphic. To fully appreciate the beauty of protein structure, you need to be able to describe each detail structure of proteins using the terms of cis and trans of peptide bond, dihedral angles of phi ( $\phi$ ) and psi ( $\psi$ ),  $\alpha$ -helix and  $\beta$ -sheet.

### Step 1

With the alpha carbon and other atoms, build a trans peptide bond followed by making the alpha carbon to L-form. We call this a basic unit. (Please note that the basic unit is not quite an amino acid)

Hint:



RS system:

Assign a priority to each group attached to a chiral carbon based upon atomic mass priority (1 highest, 4 lowest)

- If two atoms are identical, move to the next atoms
- For double or triple bonds, count atom once for each bond (-CHO higher priority than -CH<sub>2</sub>OH)
- Priorities (low to high): -H, -CH<sub>3</sub>, -C<sub>6</sub>H<sub>5</sub>, -CH<sub>2</sub>OH, -CHO, -COOH, -NH<sub>2</sub>, -NHR,

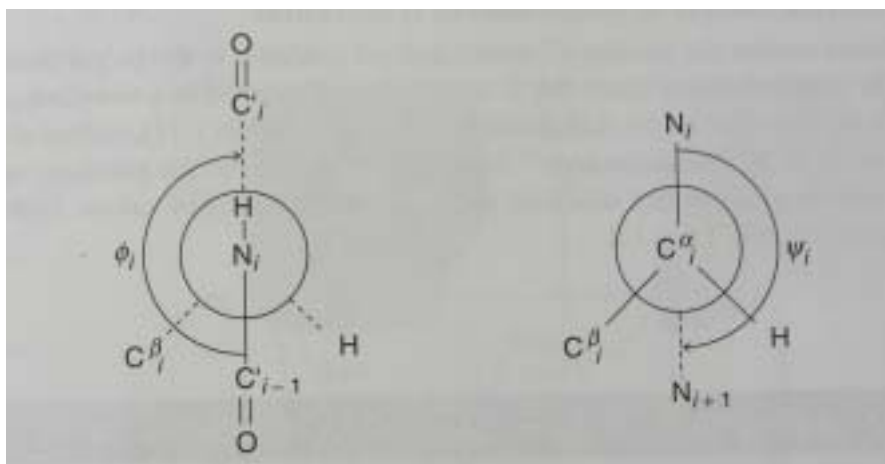
-OH, -OR, -SH

Step 2

With three L-form basic units, connect them to build a dipeptide followed by a tripeptide. Make the tripeptide to the fully extended form. It should present as  $\phi = \psi = 180^\circ$

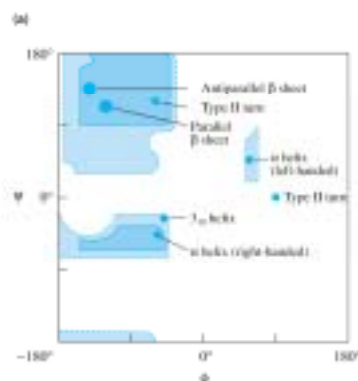
Step 3

Learn how to tell the dihedral angles.



Step 4

Make phi and psi angles for alpha helix



Step 5

Connect your tripeptide with that of your partner. Try to make the intra-chain hydrogen bond. (c=O group of residue i make H-bond with NH of residue i+4)

Step 6

Collect your tripeptide, now make a beta sheet.