Lecture 4 – Primary Structure of Amino Acids

Peptide Bond

- Two resonance structures in the peptide bond – acts to stabilise the bond
- Length of peptide bond is 1.32 angstroms – length between single and double bond
- Double bond character gives rigidity and planarity
- Plane involving α-carbon and the peptide bond – planes can swivel with respect to each other

Peptide Bond Configuration

- Peptide bonds are usually in the trans-configuration (180°) – α-carbons on opposite side of the peptide bond
- Cis-configuration (0°) when α-carbons on the same side
- Torsion angle is defined in relation to four atoms
- Trans peptide bond is more stable, as its more sterically favoured and is by far the most common (1000x more)
- Trans-proline is only slightly more stable than cis-proline (4x) – due to indole ring causing steric hindrance in both – thus cis-proline bonds are more commonly seen than other cis-configurations of amino acids – may be important in helping create a well structured protein

Primary Amino Acid Sequence (Covalent Structure)

- Primary sequence always labelled from the N-terminus to the C-terminus
- Three letter code:

Ser-Gly-Tyr-Ala-Leu

- One letter code

SYGAL

- Name of peptide

Serylglycltyrosylalanylleucine

- Thus peptides are not the same just because they have the same order of amino acids – the sequence must be going in the same direction as well
- Covalent structures of proteins also include disulphide bridges – 2 cysteines bonding together via their thiol group

Properties of Covalent Structure

- M.W. of peptides, polypeptides and proteins vary massively in their length
- Crudely calculating the mass of a peptide:

$$mass\ of\ peptide = number\ of\ amino\ acid\ residues \times 100\ Da$$

- Important to consider concentration
- Dalton (Da) – standard unit of mass for indicating mass on an atomic or molecular scale – 1 Da is equal to the mass of one nucleon and equal to 1 g/mol

Ionisation of Peptides, Polypeptides and Proteins

- pKa can vary massively within a protein
- as a peptide becomes longer the carboxylate wants to attract a proton – its pKa increases as it gets longer
- amine group wants to lose a proton as the peptide gets longer – pKa decreases as it gets longer