Conformational Angles and Properties of Ω-Amino Acids in Protein Folding

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Introduction

The conformational properties of α-amino acids are defined by three sets of torsion angles φ, ψ and ω, while in omega (ω) amino acids, due to the insertion of one or more methylene groups between the N- and Cα-atoms into the peptide backbone, the accessible conformational space is greater than α-amino acids. β-, γ-, δ-… amino acid residues belong to the family of ω-amino acids.

While significant work has been done using the alpha, and beta amino acids for the conformational transitions and their importance in the field of nanomaterials and peptide based vaccine adjuvant developments [1-7]. The angles of amino acids and their three dimensional structure play a crucial role in enhancing immune response and vaccine development [5-7].

The conformational properties of β-amino acid residues are based on three degrees of freedom: φ (N - Cβ), θ (Cβ - Cα), ψ (Cα - CO). Similarly, the conformational variabilities of γ- and δ- amino acid residues are defined as four [φ (N - Cγ), θ1 (Cγ - Cβ), θ2 (Cβ - Cα), ψ (Cα - CO)] and five [φ (N - Cδ), θ1 (Cδ - Cγ), θ2 (Cγ - Cβ), θ3 (Cβ - Cα), ψ (Cα - CO)] degrees of freedom, respectively [8]. Figure 1a illustrates the comparison of backbone torsion angles in α-, β-, γ- and δ-amino acid residues.

These torsion angles about the polymethylene chains are denoted as θ1, θ2,……θn, with increasing subscript numbers begin from N-terminus to C-terminus. The θ torsion angles lie close to gauche (θ ≈ ± 60°) or trans (θ = 180°) conformations. Conventionally for β and higher ω-amino acids the Cβ / Cω atom precedes the Cα-atom, when the chain is read from N-terminus. βGly (β-homoglycine) is the simplest member of the β-amino acid family. For example, in β-residues, when substituent takes at the Cα-carbon atom it is defined as β2 while at the Cβ-carbon atom, it is defined as β3. Figure 1b illustrates the nomenclature of acyclic substituted β-amino acid residues.

Figure 1: (a) Definition of backbone torsion angles in α, β, γ, δ and ε-amino acid residues: Gly → glycine, βGly → beta glycine, γAbu → gamma aminobutyric acid, δAva → delta aminovaleric acid and εAcp → epsilon amino caproic acid. (b) Acyclic β-amino acid residues.

Figure 2 shows the definition of β3-HAla, β3-HVal, β3-HPhe, β3-HLeu and β3-HPro residues. β3-HAla, β3-HVal, β3-HPhe, β3-HLeu and β3-HPro residues are referred in this thesis as βAla, βVal, βPhe, βLeu and βPro, respectively. γAbu (gamma aminobutyric acid) and δAva (delta aminovaleric acid) are the simplest members of the γ- and δ-families, respectively.
Currently, small molecule based drug increasingly interest in development of anti-cancer therapy molecules like Bortezomib, gold nanoparticles platinum based inorganic molecules for anti-tumor therapy [9]. The homologation alpha amino acids to beta amino acids or gamma amino acids would enhance the penetration of drug molecules inside the cellular lever to develop the anticancer drugs. The incorporation of inorganic drug molecules co-ordination with protein secondary structures would help for development for vaccines for cancer treatment [10,11].

References