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A cross sectional study done on various dipeptides and tripeptides containing cysteine: DFTapproach

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Case Study: Density Functional Theory (DFT) calculations have been carried out on a series of thirty two dipeptides and eleven tripeptides. Dipeptides were constructed by fixing cysteine at N-terminus/C-terminus and varying the remaining terminus with sixteen different amino acids: *alanine(Ala), arginine(Arg), asparagine(Asn), cysteine(Cys), glutamine(Gln), glycine(Gly), isoleucine(Ile), leucine(Leu), lysine(Lys), Methionine(Met), phenylalanine(Phe), serine(Ser), threonine(Thr), tryptophan(Trp), tyrosine(Tyr) and valine(Val)*. To study the structural stability and sequence of amino acids in dipeptides and tripeptides, we have investigated the bond lengths and bond angles of amide plane.The analysis of α-carbon bond angle resulted that the bond angle around the α-carbon of cysteine residue does not vary significantly, as only a max- imum deviation of 0.4° is seen in the case of dipeptide, but the bond angle around the α-carbon of varied amino acids shows a significant deviation, the maximum deviation be- ing 3.3° in Cys-Gly combination. And, the bond angle around the α-carbon of tripeptide shows the significant deviation in the α-carbon bond angle of X- and Y-amino group, being maximum deviation of 3.0° and 3.2° for each group in Cys-Cys-Gln and Gln-Cys-Gly re- spectively. In conclusion, there is deviation of amide plane from planarity, which is drawn from the investigation of dihedral angle analysis of dipeptides and tripeptides. In order to study internal barriers to the rotation, we have performed the potential energy scan of the optimized structure of cysteine residue by rotating three different groups separately: (a) amino (-NH_2) group (b) carboxyl (-COOH) group and (c)-R (-CH_2SH) group. The value of energy barrier for the lowest energy conformers after the rotation of -NH_2, -COOH and -R group are obtained to be 4.708 kcal mol^{-1}, 3.625 kcal mol^{-1} and 5.879 kcal mol^{-1} respectively.