Evaluations of Force Field Parameters for D-Amino Acid Residues Using Density Functional Theory

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In the past, proteins in the living body were considered to be constructed only of L-amino acids. However, D-amino acids have recently been reported in living mammals; some proteins are known to contain D-amino acids as residues. In this study, molecular mechanics (MM) force field parameters of D-amino acids were evaluated for the simulations of proteins including D-amino acids. In order to evaluate force field parameters of D-amino acids, nonapeptide AAAAXAAAA (A: L-alanine, X: D-amino acid) were computationally constructed, and the energies of the nonapeptide calculated by MM were compared with the energies calculated by B3LYP/6-31G*. For comparison, the energies of L-amino acid peptide AAAAX′AAAA (X′: L-amino acid) were also calculated.

For the nonapeptide, more than 200 conformers were generated, and conformational energies of them were calculated. The correlation coefficients between energies obtained by MM (E_{MM}) and those by DFT calculation (E_{QM}) for D-amino acid peptide were similar to that for L-amino acid peptide. The results indicate that same parameters can be used for D-amino acids and L-amino acids.