Evaluations of Density Functionals and Solvation Effect for Racemization Reaction of Amino Acid Residues

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In the past, proteins in the living body were considered to be constructed only of L-amino acids. Actually, the majority of proteins are built from L-amino acids. However, based on recent developments in analytical sciences and technologies, various D-amino acids have been widely found in mammals, including human beings, and have revealed a physiological function. The D-amino acid residues are presumed to be one of the causes for the several diseases, such as Alzheimer's dementia and cataract, and the stereoinversions of amino acid residues in proteins may cause the age-related diseases. Recently, we have studied the reaction pathway of D-Asp residues, which is chiefly founded D-amino acid residue, using the density functional theory (B3LYP/6-31+G(d,p)) However the influence of density functionals were not investigated sufficiently. In this study, we calculated the optimized structure and activation energy of the racemization reaction using the B3LYP, B3LYP-D3, CAM-B3LYP, PBEPBE, M06-2X, ωB97XD, B3PW91, TPSSTPSS, mPW1PW91, HSEh1PBE, HCTH and BVP86 density functional methods for model compounds and compared with each other.