Application of MDR to the analysis of molecular hydrodynamic property

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One of the widespread methodologies to describe the molecular surface shape is the spherical harmonic expansion. However, these techniques are needed the pre-processing of MSP or MSMS to calculate the expansion coefficients. We presented more efficient approach to describe the shape of globular protein molecular surface analytically by using the Multipole Deformation Representation (MDR) commonly employed for the parameterization of nuclear surface. In MDR method, the radial coordinate of a protein surface can be expressed as a sum of multipole moments of the deformation relative to a reference spherical surface. We used the multipoles up to the dotriacontapole moment equivalent to the 5-th order of spherical harmonic expansion to describe the protein molecular surface of lysozyme.
Further more we calculate the hydrodynamic radius of protein molecule by using the MDR method. Monopole moment of shape function is employed as correlation parameter of hydrodynamic radius. MDR method also furnishes a reasonably accurate estimation for the hydrodynamic radius of protein molecule that well correlates with the translational diffusivity measurement data.