Analytical surface representation for protein molecules: Application I. Calculation of the hydrodynamic radius for protein molecules

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The surface of protein can e expressed in terms of the radial coordinates of the surface point. In this work, we obtained the surface shape of protein molecules by using the multipole deformation representation which describes the deformation from the spherical shape. The deformation is also expressed as a sum of the spherical surface harmonics. We take into account of the surface harmonics of degrees up to 5. The corresponding coefficients are monopole, dipole, quadrupole, octupole, hexadecapole, and dotriacontapole. For protein molecules, the coefficients can be obtained from the surface integration over a unit sphere. Furthermore, we obtained analytical representation of the surface area and volume for protein molecules.

One of the application of this work, we calculate the hydrodynamic radius of protein molecules from the surface obtained by the multipole deformation representation. For the calculation of the hydrodynamic mobility tensor we use a Fredholm integral equation of the second kind and compare the results with earlier experimental values that derived from the Stokes-Einstein equation.