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Estimation of the internal dielectric constant of proteins using measured and simulated charge moments BRETT MELLOR, EFREN CRUZ CORTES, DAVID BUSATH, BRIAN MAZZEO, Brigham Young University — Protein structure, function, and interaction are, in part, a consequence of the low permittivity region surrounding the hydrophobic core of the molecule. We present a novel approach to estimate the dielectric constant of this region using measured and simulated first- and second-order charge moments. The second-order moment, the dipole moment, is measured using dielectric spectroscopy in a temperature-stable parallel-plate cell. The first-order moment, overall charge, and the dipole moment are calculated using structures from the Protein Data Bank and refined structures using molecular dynamics in CHARMM. The best estimate is evaluated in terms of the dielectric constant that minimizes the root mean square residual between measured and simulated charge moments. This method is carried out on the protein β-lactoglobulin, for which a dielectric constant in the range of 6 to 7 is estimated.

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