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Using DelPhi capabilities to mimic conformational reorganization with amino acid specific dielectric constants[1] LIN WANG, Clemson University, SUBHRA SARHAR, Clemson, WALTER ROCCHIA, Italian Institute of Technology, EMIL ALEXOV, Clemson University — Many molecular events are associated with small or large conformational changes occurring in the corresponding proteins. Modeling such changes is a challenge and requires significant amount of computing time. From point of view of electrostatics, these changes can be viewed as a reorganization of local charges and dipoles in response to the changes of the electrostatic field, if the cause is insertion or deletion of a charged amino acid. Here we report a large scale investigation of modeling the changes of the folding energy due to single mutations involving charge group. This allows the changes of the folding energy to be considered mostly electrostatic in origin and to be calculated with DelPhi assigning residue-specific value of the internal dielectric constant of protein in the range from 2 to 20. The predicted energy changes are benchmarked against experimentally measured changes of the folding energy on a set of 300 single mutations. The best fit between experimental values and predicted changes is used to find out the effective value of the internal dielectric constant for each type of amino acid.

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