

Abstract Submitted  
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**Rigorous surface charge method for determining electrostatic interaction energies in biomolecular systems**<sup>1</sup> T.P. DOERR, O.I. BOLENSKY, A.Y. OGURTSOV, YI-KUO YU, National Center for Biotechnology Information/NIH — Classical electrostatics plays a crucial role in biomolecular systems, dominating the interactions that determine the formation and dissolution of complexes responsible for the operation of cells. For systems that can be modeled as a set of piecewise-constant dielectric bodies, surface charge methods are usually preferable in both analytical and numerical contexts. We present a numerical implementation of a surface charge method previously used in analytical contexts. The method is applied to a realistic model of trypsin, an important protein involved in digesting other proteins, and one of its inhibitors, benzamidine. The classical calculations are complemented by density function theory calculations at short separations for which the classical model is inappropriate. We find that the surface charge method correctly distinguishes between correct and incorrect docking sites.

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