Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

DelPhi webserver: Comprehensive suite for electrostatic calculations of biological macromolecules and their complexes SHAWN WITHAM, BRETT BOYLEN, BARR OWESEN, Clemson University, WALTER ROCCHIA, Italian Institute of Technology, EMIL ALEXOV, Clemson University — Electrostatic forces and energies are two of the major components that contribute to the stability, function and interaction of biological macromolecules. The calculations of the electrostatic potential distribution in such systems, which are comprised of irregularly shaped objects immersed in a water phase, is not a trivial task. In addition, an accurate model requires any missing hydrogen atoms of the corresponding structural files (Protein Data Bank, or, PDB files) to be generated in silico and, if necessary, missing atoms or residues to be predicted as well. Here we report a comprehensive suite, an academic DelPhi webserver, which allows the users to upload their structural file, calculate the components of the electrostatic energy, generate the corresponding potential (and/or concentration/dielectric constant) distribution map, and choose the appropriate force field. The webserver utilizes modern technology to take user input and construct an algorithm that suits the users specific needs. The webserver uses Clemson University's Palmetto Supercomputer Cluster to handle the DelPhi calculations, which can range anywhere from small and short computation times, to extensive and computationally demanding runtimes. The work was supported by a grant from NIGMS, NIH, grant number 1R01GM093937-01.

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Date submitted: 17 Nov 2010 Electronic form version 1.4