Marcia O Fenley

List of Publications by Year
in descending order

36	1,201	361413	395702
papers	citations	20 h-index	33 g-index

36	36	36	1032
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Accuracy Comparison of Generalized Born Models in the Calculation of Electrostatic Binding Free Energies. Journal of Chemical Theory and Computation, 2018, 14, 1656-1670.	5.3	23
2	Numerical Difficulties Computing Electrostatic Potentials Near Interfaces with the Poissonâ€“Boltzmann Equation. Journal of Chemical Theory and Computation, 2017, 13, 3945-3951.	5.3	3
3	Problems of Robustness in Poissonâ€“Boltzmann Binding Free Energies. Journal of Chemical Theory and Computation, 2015, 11, 705-712.	5.3	14
4	Features of CPB: A <scp>P</scp>oissonâ€“<scp>B</scp>oltzmann solver that uses an adaptive cartesian grid. Journal of Computational Chemistry, 2015, 36, 235-243.	3.3	4
5	A Comprehensive Exploration of Physical and Numerical Parameters in the Poissonâ€“Boltzmann Equation for Applications to Receptorâ€“Ligand Binding. , 2015, , 39-71.		5
6	The Adaptive Cartesian Grid-Based Poissonâ€“Boltzmann Solver: Energy and Surface Electrostatic Properties. , 2015, , 73-110.		3
7	Sensitivities to parameterization in the size-modified Poisson-Boltzmann equation. Journal of Chemical Physics, 2014, 140, 075102.	3.0	25
8	Excluded volume and ion-ion correlation effects on the ionic atmosphere around B-DNA: Theory, simulations, and experiments. Journal of Chemical Physics, 2014, 141, 225103.	3.0	24
9	Influence of Grid Spacing in Poissonâ€“Boltzmann Equation Binding Energy Estimation. Journal of Chemical Theory and Computation, 2013, 9, 3677-3685.	5.3	29
10	Numerical Optimization of a Walk-on-Spheres Solver for the Linear Poisson-Boltzmann Equation. Communications in Computational Physics, 2013, 13, 195-206.	1.7	12
11	A Stochastic Solver of the Generalized Born Model. Computational and Mathematical Biophysics, 2013, 1, 63-74.	1.1	6
12	The Ionic Atmosphere around A-RNA: Poisson-Boltzmann and Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 829-838.	0.5	68
13	Theoretical Assessment of the Oligolysine Model for Ionic Interactions in Proteinâ€“DNA Complexes. Journal of Physical Chemistry B, 2011, 115, 9864-9872.	2.6	30
14	A Fast and Robust Poissonâ€“Boltzmann Solver Based on Adaptive Cartesian Grids. Journal of Chemical Theory and Computation, 2011, 7, 1524-1540.	5.3	51
15	Understanding the physical basis of the salt dependence of the electrostatic binding free energy of mutated charged ligandâ€“nucleic acid complexes. Biophysical Chemistry, 2011, 156, 79-87.	2.8	14
16	DNAâ€“ Drug Interactions. , 2011, , .		4
17	Revisiting the Association of Cationic Groove-Binding Drugs to DNA Using a Poisson-Boltzmann Approach. Biophysical Journal, 2010, 99, 879-886.	0.5	28
18	Using Correlated Monte Carlo Sampling for Efficiently Solving the Linearized Poissonâ^'Boltzmann Equation Over a Broad Range of Salt Concentration. Journal of Chemical Theory and Computation, 2010, 6, 300-314.	5.3	12

#	Article	IF	Citations
19	Comparing the Predictions of the Nonlinear Poissonâ^'Boltzmann Equation and the Ion Size-Modified Poissonâ^'Boltzmann Equation for a Low-Dielectric Charged Spherical Cavity in an Aqueous Salt Solution. Journal of Chemical Theory and Computation, 2010, 6, 3631-3639.	5.3	35
20	Properties of the nucleic-acid bases in free and Watson-Crick hydrogen-bonded states: computational insights into the sequence-dependent features of double-helical DNA. Biophysical Reviews, 2009, 1, 13-20.	3.2	35
21	Efficient sampling of ion motions in molecular dynamics simulations on DNA: Variant Hamiltonian replica exchange method. Chemical Physics Letters, 2008, 454, 391-395.	2.6	15
22	Salt-Mediated Electrostatics in the Association of TATA Binding Proteins to DNA: A Combined Molecular Mechanics/Poisson-Boltzmann Study. Biophysical Journal, 2008, 94, 4634-4645.	0.5	20
23	Proteinâ^'Ion Binding Process on Finite Macromolecular Concentration. A Poissonâ^'Boltzmann and Monte Carlo Study. Journal of Physical Chemistry B, 2008, 112, 16766-16776.	2.6	13
24	The electrostatic characteristics of G{middle dot}U wobble base pairs. Nucleic Acids Research, 2007, 35, 3836-3847.	14.5	38
25	Monte Carlo-based linear Poisson-Boltzmann approach makes accurate salt-dependent solvation free energy predictions possible. Journal of Chemical Physics, 2007, 127, 185105.	3.0	22
26	A new outer boundary formulation and energy corrections for the nonlinear Poissonâ€“Boltzmann equation. Journal of Computational Chemistry, 2007, 28, 909-921.	3.3	42
27	Recognition of the spliceosomal branch site RNA helix on the basis of surface and electrostatic features. Nucleic Acids Research, 2005, 33, 1154-1161.	14.5	18
28	Structural and Thermodynamic Evidence for a Stabilizing Role of Nop5p in S-Adenosyl-L-methionine Binding to Fibrillarin. Journal of Biological Chemistry, 2004, 279, 41822-41829.	3.4	28
29	Molecular Basis of Box C/D RNA-Protein Interactions. Structure, 2004, 12, 807-818.	3.3	158
30	Impact of a Poissonâ€“Boltzmann electrostatic restraint on protein structures refined at medium resolution. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 1786-1794.	2.5	6
31	Hybrid boundary element and finite difference method for solving the nonlinear Poisson-Boltzmann equation. Journal of Computational Chemistry, 2004, 25, 935-955.	3.3	88
32	Fast Boundary Element Method for the Linear Poissonâ^'Boltzmann Equation. Journal of Physical Chemistry B, 2002, 106, 2741-2754.	2.6	144
33	A Fast Adaptive Multipole Algorithm for Calculating Screened Coulomb (Yukawa) Interactions. Journal of Computational Physics, 1999, 151, 212-241.	3.8	35
34	Fast adaptive multipole method for computation of electrostatic energy in simulations of polyelectrolyte DNA. Journal of Computational Chemistry, 1996, 17, 976-991.	3.3	32
35	Approach to the limit of counterion condensation. Biopolymers, 1990, 30, 1191-1203.	2.4	99
36	A numerical counterion condensation analysis of the B-Z transition of DNA. Biopolymers, 1990, 30, 1205-1213.	2.4	18