George A Kaminski

List of Publications by Year
in descending order

30 papers	5,605 citations	448610 19 h-index	536525 29 g-index
30 all docs	30 docs citations	30 times ranked	8000 citing authors

#	Article	IF	Citations
1	Expansion and Additional Validation of PKA17: A Fast Real-Time and Web-Based pKa Predictor. Journal of Computational Biophysics and Chemistry, 2021, 20, 141-152.	1.0	2
2	PKA17â€"A Coarseâ€Grain Gridâ€Based Methodology and Webâ€Based Software for Predicting Protein pK_a Shifts. Journal of Computational Chemistry, 2019, 40, 1718-1726.	1.5	17
3	Binding of Copper and Cisplatin to Atox1 Is Mediated by Glutathione through the Formation of Metalâ€"Sulfur Clusters. Biochemistry, 2017, 56, 3129-3141.	1.2	27
4	Using polarizable POSSIM force field and fuzzyâ€border continuum solvent model to calculate pK_a shifts of protein residues. Journal of Computational Chemistry, 2017, 38, 65-80.	1.5	3
5	Developing multisite empirical force field models for Pt(II) and cisplatin. Journal of Computational Chemistry, 2017, 38, 161-168.	1.5	5
6	POSSIM: Parameterizing Complete Second-Order Polarizable Force Field for Proteins. Journal of Chemical Theory and Computation, 2014, 10, 4896-4910.	2.3	10
7	Computational Studies of the Effect of Shock Waves on the Binding of Model Complexes. Journal of Chemical Theory and Computation, 2014, 10, 4972-4981.	2.3	3
8	Polarizable simulations with second order interaction model (POSSIM) force field: Developing parameters for protein sideâ€chain analogues. Journal of Computational Chemistry, 2013, 34, 1241-1250.	1.5	10
9	Effects of Lysine Substitution on Stability of Polyalanine Î± Helix. Journal of Chemical Theory and Computation, 2012, 8, 4691-4706.	2.3	8
10	Calculating pK_a values for substituted phenols and hydration energies for other compounds with the firstâ€order fuzzyâ€border continuum solvation model. Journal of Computational Chemistry, 2012, 33, 2388-2399.	1.5	23
11	Importance of electrostatic polarizability in calculating cysteine acidity constants and copper(I) binding energy of Bacillus subtilis CopZ. Journal of Computational Chemistry, 2012, 33, 1142-1151.	1.5	15
12	Electrostatic Polarization Is Crucial in Reproducing Cu(I) Interaction Energies and Hydration. Journal of Physical Chemistry B, 2011, 115, 10079-10085.	1.2	15
13	Polarizable Simulations with Second-Order Interaction Model (POSSIM) Force Field: Developing Parameters for Alanine Peptides and Protein Backbone. Journal of Chemical Theory and Computation, 2011, 7, 1415-1427.	2.3	19
14	Quality of random number generators significantly affects results of Monte Carlo simulations for organic and biological systems. Journal of Computational Chemistry, 2011, 32, 513-524.	1.5	31
15	Polarizable Simulations with Second-Order Interaction Modelâ€"Force Field and Software for Fast Polarizable Calculations: Parameters for Small Model Systems and Free Energy Calculations. Journal of Chemical Theory and Computation, 2009, 5, 2935-2943.	2.3	26
16	Reproducing Basic pK_a Values for Turkey Ovomucoid Third Domain Using a Polarizable Force Field. Journal of Physical Chemistry B, 2009, 113, 7844-7850.	1.2	20
17	Electrostatic Polarization Is Crucial for Reproducing pKa Shifts of Carboxylic Residues in Turkey Ovomucoid Third Domain. Journal of Physical Chemistry B, 2007, 111, 9036-9044.	1.2	34
18	Pseudospectral Local Second-Order MÃ¸llerâ€"Plesset Methods for Computation of Hydrogen Bonding Energies of Molecular Pairs. Journal of Chemical Theory and Computation, 2005, 1, 248-254.	2.3	32

#	Article	IF	Citations
19	Accurate Prediction of Absolute Acidity Constants in Water with a Polarizable Force Field:Â Substituted Phenols, Methanol, and Imidazole. Journal of Physical Chemistry B, 2005, 109, 5884-5890.	1.2	48
20	A Polarizable Force Field and Continuum Solvation Methodology for Modeling of Proteinâ"Ligand Interactions. Journal of Chemical Theory and Computation, 2005, 1, 694-715.	2.3	100
21	Development of an Accurate and Robust Polarizable Molecular Mechanics Force Field from ab Initio Quantum Chemistry. Journal of Physical Chemistry A, 2004, 108, 621-627.	1.1	221
22	A computationally inexpensive modification of the point dipole electrostatic polarization model for molecular simulations. Journal of Computational Chemistry, 2003, 24, 267-276.	1.5	56
23	Force Field Validation Using Protein Side Chain Prediction. Journal of Physical Chemistry B, 2002, 106, 11673-11680.	1.2	165
24	Development of a polarizable force field for proteins via ab initio quantum chemistry: First generation model and gas phase tests. Journal of Computational Chemistry, 2002, 23, 1515-1531.	1.5	296
25	Evaluation and Reparametrization of the OPLS-AA Force Field for Proteins via Comparison with Accurate Quantum Chemical Calculations on Peptidesâ€. Journal of Physical Chemistry B, 2001, 105, 6474-6487.	1.2	3,513
26	Parametrizing a polarizable force field from ab initio data. I. The fluctuating point charge model. Journal of Chemical Physics, 1999, 110, 741-754.	1.2	251
27	A Quantum Mechanical and Molecular Mechanical Method Based on CM1A Charges:â€‰ Applications to Solvent Effects on Organic Equilibria and Reactions. Journal of Physical Chemistry B, 1998, 102, 1787-1796.	1.2	113
28	Performance of the AMBER94, MMFF94, and OPLS-AA Force Fields for Modeling Organic Liquids. The Journal of Physical Chemistry, 1996, 100, 18010-18013.	2.9	242
29	Free Energies of Hydration and Pure Liquid Properties of Hydrocarbons from the OPLS All-Atom Model. The Journal of Physical Chemistry, 1994, 98, 13077-13082.	2.9	300
30	Expansion and additional validation of PKA17: A fast real-time and web-based pKa predictor. Journal of Theoretical and Computational Chemistry, 0, , 2042003.	1.8	0