Adrian H Elcock

List of Publications by Year
in descending order

82 papers	5,838 citations	76326 40 h-index	76900 74 g-index
89 all docs	89 docs citations	89 times ranked	6314 citing authors

#	Article	IF	Citations
1	Diffusion, Crowding & Protein Stability in a Dynamic Molecular Model of the Bacterial Cytoplasm. PLoS Computational Biology, 2010, 6, e1000694.	3.2	612
2	Physicochemical Properties of Cells and Their Effects on Intrinsically Disordered Proteins (IDPs). Chemical Reviews, 2014, 114, 6661-6714.	47.7	391
3	The stability of salt bridges at high temperatures: implications for hyperthermophilic proteins 1 1Edited by B. Honig. Journal of Molecular Biology, 1998, 284, 489-502.	4.2	295
4	Models of macromolecular crowding effects and the need for quantitative comparisons with experiment. Current Opinion in Structural Biology, 2010, 20, 196-206.	5.7	257
5	The Native 3D Organization of Bacterial Polysomes. Cell, 2009, 136, 261-271.	28.9	240
6	Computer Simulation of Proteinâ^'Protein Interactions. Journal of Physical Chemistry B, 2001, 105, 1504-1518.	2.6	203
7	Electrostatic contributions to the stability of halophilic proteins. Journal of Molecular Biology, 1998, 280, 731-748.	4.2	202
8	Prediction of functionally important residues based solely on the computed energetics of protein structure 1 1Edited by B. Honig. Journal of Molecular Biology, 2001, 312, 885-896.	4.2	195
9	Computer simulation of protein-protein association kinetics: acetylcholinesterase-fasciculin. Journal of Molecular Biology, 1999, 291, 149-162.	4.2	181
10	Molecular Dynamics Simulations of Hydrophobic Associations in Aqueous Salt Solutions Indicate a Connection between Water Hydrogen Bonding and the Hofmeister Effect. Journal of the American Chemical Society, 2007, 129, 14887-14898.	13.7	151
11	Computing ionization states of proteins with a detailed charge model. Journal of Computational Chemistry, 1996, 17, 1633-1644.	3.3	139
12	Toward Optimized Potential Functions for Proteinâ€"Protein Interactions in Aqueous Solutions: Osmotic Second Virial Coefficient Calculations Using the MARTINI Coarse-Grained Force Field. Journal of Chemical Theory and Computation, 2013, 9, 4176-4185.	5.3	120
13	Identification of protein oligomerization states by analysis of interface conservation. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 2990-2994.	7.1	107
14	Striking Effects of Hydrodynamic Interactions on the Simulated Diffusion and Folding of Proteins. Journal of Chemical Theory and Computation, 2009, 5, 242-256.	5.3	106
15	Molecular Simulations of Cotranslational Protein Folding: Fragment Stabilities, Folding Cooperativity, and Trapping in the Ribosome. PLoS Computational Biology, 2006, 2, e98.	3.2	105
16	Atomically Detailed Simulations of Concentrated Protein Solutions:Â The Effects of Salt, pH, Point Mutations, and Protein Concentration in Simulations of 1000-Molecule Systems. Journal of the American Chemical Society, 2006, 128, 12098-12110.	13.7	97
17	Computational Sampling of a Cryptic Drug Binding Site in a Protein Receptor: Explicit Solvent Molecular Dynamics and Inhibitor Docking to p38 MAP Kinase. Journal of Molecular Biology, 2006, 359, 202-214.	4.2	91
18	Realistic modeling of the denatured states of proteins allows accurate calculations of the ph dependence of protein stability. Journal of Molecular Biology, 1999, 294, 1051-1062.	4.2	90

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19	Calculation of Weak Protein-Protein Interactions: The pH Dependence of the Second Virial Coefficient. Biophysical Journal, 2001, 80, 613-625.	0.5	90
20	Human Heterochromatin Protein 1Î± Promotes Nucleosome Associations That Drive Chromatin Condensation. Journal of Biological Chemistry, 2014, 289, 6850-6861.	3.4	86
21	Stacking Free Energies of All DNA and RNA Nucleoside Pairs and Dinucleoside-Monophosphates Computed Using Recently Revised AMBER Parameters and Compared with Experiment. Journal of Chemical Theory and Computation, 2015, 11, 2315-2328.	5.3	86
22	Molecular Simulations Suggest Protein Salt Bridges Are Uniquely Suited to Life at High Temperatures. Journal of the American Chemical Society, 2004, 126, 2208-2214.	13.7	83
23	Sequence Selective Binding to the DNA Major Groove: Tris(1,10-phenanthroline) Metal Complexes Binding to Poly(dG-dC) and Poly(dA-dT). Journal of Biomolecular Structure and Dynamics, 1991, 9, 23-44.	3.5	82
24	Dynamic binding of replication protein a is required for DNA repair. Nucleic Acids Research, 2016, 44, 5758-5772.	14.5	82
25	Electrostatic Channeling in the Bifunctional Enzyme Dihydrofolate Reductase-thymidylate Synthase. Journal of Molecular Biology, 1996, 262, 370-374.	4.2	73
26	Absolute Protein-Protein Association Rate Constants from Flexible, Coarse-Grained Brownian Dynamics Simulations: The Role of Intermolecular Hydrodynamic Interactions in Barnase-Barstar Association. Biophysical Journal, 2010, 99, L75-L77.	0.5	72
27	Evidence for Electrostatic Channeling in a Fusion Protein of Malate Dehydrogenase and Citrate Synthaseâ€. Biochemistry, 1996, 35, 12652-12658.	2.5	70
28	Computer simulations of actin polymerization can explain the barbed-pointed end asymmetry. Journal of Molecular Biology, 1999, 294, 1181-1189.	4.2	65
29	The Low Dielectric Interior of Proteins is Sufficient To Cause Major Structural Changes in DNA on Association. Journal of the American Chemical Society, 1996, 118, 3787-3788.	13.7	64
30	Electrostatic Channeling of Substrates between Enzyme Active Sites:â€‰ Comparison of Simulation and Experiment. Biochemistry, 1997, 36, 16049-16058.	2.5	64
31	Rapid binding of a cationic active site inhibitor to wild type and mutant mouse acetylcholinesterase: Brownian dynamics simulation including diffusion in the active site gorge. Biopolymers, 1998, 46, 465-474.	2.4	58
32	Atomic-level observation of macromolecular crowding effects: Escape of a protein from the GroEL cage. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 2340-2344.	7.1	58
33	Electrostatic effects in homeodomain-DNA interactions. Journal of Molecular Biology, 1997, 267, 368-381.	4.2	52
34	Dynamics and Energy Contributions for Transport of Unfolded Pertactin through a Protein Nanopore. ACS Nano, 2015, 9, 9050-9061.	14.6	52
35	Structure Selection for Protein Kinase Docking and Virtual Screening:Homology Models or Crystal Structures?. Current Protein and Peptide Science, 2006, 7, 437-457.	1.4	51
36	Rapid Computational Identification of the Targets of Protein Kinase Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 4138-4152.	6.4	50

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37	Continuum Solvation Model for Studying Protein Hydration Thermodynamics at High Temperatures. Journal of Physical Chemistry B, 1997, 101, 9624-9634.	2.6	49
38	Optimizing Soluteâ€“Solute Interactions in the GLYCAM06 and CHARMM36 Carbohydrate Force Fields Using Osmotic Pressure Measurements. Journal of Chemical Theory and Computation, 2016, 12, 1401-1407.	5.3	48
39	Features of genomic organization in a nucleotide-resolution molecular model of the Escherichia coli chromosome. Nucleic Acids Research, 2017, 45, 7541-7554.	14.5	48
40	Direct Observation of Salt Effects on Molecular Interactions through Explicit-Solvent Molecular Dynamics Simulations:Â Differential Effects on Electrostatic and Hydrophobic Interactions and Comparisons to Poissonâ^'Boltzmann Theory. Journal of the American Chemical Society, 2006, 128, 7796-7806.	13.7	45
41	Combined Quantum and Molecular Mechanical Study of DNA Crosslinking by Nitrous Acid. Journal of the American Chemical Society, 1995, 117, 4706-4707.	13.7	43
42	Cotranslational protein assembly imposes evolutionary constraints on homomeric proteins. Nature Structural and Molecular Biology, 2018, 25, 279-288.	8.2	43
43	Progress toward virtual screening for drug side effects. Proteins: Structure, Function and Bioinformatics, 2002, 48, 664-671.	2.6	38
44	Computer simulations of the bacterial cytoplasm. Biophysical Reviews, 2013, 5, 109-119.	3.2	37
45	Reparametrization of Protein Force Field Nonbonded Interactions Guided by Osmotic Coefficient Measurements from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2017, 13, 1812-1826.	5.3	37
46	Molecular Dynamics Simulations of Highly Crowded Amino Acid Solutions: Comparisons of Eight Different Force Field Combinations with Experiment and with Each Other. Journal of Chemical Theory and Computation, 2013, 9, 4585-4602.	5.3	36
47	Relative hydration free energies of nucleic acid bases. Journal of the American Chemical Society, 1993, 115, 7930-7931.	13.7	31
48	Molecular Simulations of Diffusion and Association in Multimacromolecular Systems. Methods in Enzymology, 2004, 383, 166-198.	1.0	29
49	Reparameterization of Soluteâ€”Solute Interactions for Amino Acidâ€“Sugar Systems Using Isopiestic Osmotic Pressure Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2017, 13, 1874-1882.	5.3	29
50	Direct Measurement of the Kinetics and Thermodynamics of Association of Hydrophobic Molecules from Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2011, 2, 19-24.	4.6	28
51	Osmotic Pressure Simulations of Amino Acids and Peptides Highlight Potential Routes to Protein Force Field Parameterization. Journal of Physical Chemistry B, 2016, 120, 8217-8229.	2.6	28
52	Sequence Dependent Hydration of DNA: Theoretical Results. Journal of the American Chemical Society, 1995, 117, 10161-10162.	13.7	27
53	Residue-Specific Force Field (RSFF2) Improves the Modeling of Conformational Behavior of Peptides and Proteins. Journal of Physical Chemistry Letters, 2015, 6, 2127-2133.	4.6	26
54	Identification of Iron-Sulfur (Fe-S) Cluster and Zinc (Zn) Binding Sites Within Proteomes Predicted by DeepMindâ€™s AlphaFold2 Program Dramatically Expands the Metalloproteome. Journal of Molecular Biology, 2022, 434, 167377.	4.2	26

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55	A Complete Thermodynamic Characterization of Electrostatic and Hydrophobic Associations in the Temperature Range 0 to 100 Â°C from Explicit-Solvent Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2010, 6, 1293-1306.	5.3	25
56	Direct Comparison of Amino Acid and Salt Interactions with Double-Stranded and Single-Stranded DNA from Explicit-Solvent Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2017, 13, 1794-1811.	5.3	22
57	Large-Scale Analysis of 48 DNA and 48 RNA Tetranucleotides Studied by 1 Î¼s Explicit-Solvent Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 5906-5917.	5.3	20
58	p38Î± Mitogen-Activated Protein Kinase Is a Druggable Target in Pancreatic Adenocarcinoma. Frontiers in Oncology, 2019, 9, 1294.	2.8	20
59	Modeling supramolecular assemblages. Current Opinion in Structural Biology, 2002, 12, 154-160.	5.7	19
60	Accurate Calculation of Mutational Effects on the Thermodynamics of Inhibitor Binding to p38Î± MAP Kinase: A Combined Computational and Experimental Study. Journal of Chemical Theory and Computation, 2013, 9, 3151-3164.	5.3	18
61	A Binding Mode of A-[tris(1,10-phenanthroline)ruthenium(II)]²⁺Exhibiting Preference for Purine-3â€²,5â€²-Pyrimidine Sites of DNA. Journal of Biomolecular Structure and Dynamics, 1991, 9, 553-569.	3.5	17
62	A PEGâ€Based Oligomer as a Backbone Replacement for Surfaceâ€Exposed Loops in a Protein Tertiary Structure. ChemBioChem, 2012, 13, 1107-1111.	2.6	17
63	Flexibility of the Bacterial Chaperone Trigger Factor in Microsecond-Timescale Molecular Dynamics Simulations. Biophysical Journal, 2013, 105, 732-744.	0.5	17
64	The C-terminal region of translesion synthesis DNA polymerase Î· is partially unstructured and has high conformational flexibility. Nucleic Acids Research, 2018, 46, 2107-2120.	14.5	17
65	Mechanism of action of antifreeze polypeptide HPLC6 in solution: analysis of solvent behaviour by molecular dynamics. Chemical Physics, 1996, 204, 251-261.	1.9	16
66	Association Lifetimes of Hydrophobic Amino Acid Pairs Measured Directly from Molecular Dynamics Simulations. Journal of the American Chemical Society, 2003, 125, 13968-13969.	13.7	16
67	Proton transfer dynamics of GART: The pH-dependent catalytic mechanism examined by electrostatic calculations. Protein Science, 2008, 10, 2379-2392.	7.6	16
68	COFFDROP: A Coarse-Grained Nonbonded Force Field for Proteins Derived from All-Atom Explicit-Solvent Molecular Dynamics Simulations of Amino Acids. Journal of Chemical Theory and Computation, 2014, 10, 5178-5194.	5.3	16
69	Parametrization of Backbone Flexibility in a Coarse-Grained Force Field for Proteins (COFFDROP) Derived from All-Atom Explicit-Solvent Molecular Dynamics Simulations of All Possible Two-Residue Peptides. Journal of Chemical Theory and Computation, 2015, 11, 2341-2354.	5.3	16
70	Atomistic Simulations of Competition between Substrates Binding to an Enzyme. Biophysical Journal, 2002, 82, 2326-2332.	0.5	15
71	Native-state conformational dynamics of GART: A regulatory pH-dependent coil-helix transition examined by electrostatic calculations. Protein Science, 2008, 10, 2363-2378.	7.6	15
72	Molecular Dynamics Simulations of 441 Two-Residue Peptides in Aqueous Solution: Conformational Preferences and Neighboring Residue Effects with the Amber ff99SB-ildn-NMR Force Field. Journal of Chemical Theory and Computation, 2015, 11, 1315-1329.	5.3	13

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73	Molecule-Centered Method for Accelerating the Calculation of Hydrodynamic Interactions in Brownian Dynamics Simulations Containing Many Flexible Biomolecules. Journal of Chemical Theory and Computation, 2013, 9, 3224-3239.	5.3	11
74	Molecular chaperones: providing a safe place to weather a midlife protein-folding crisis. Nature Structural and Molecular Biology, 2016, 23, 621-623.	8.2	9
75	Molecular Dynamics Simulations Predict a Favorable and Unique Mode of Interaction between Lithium (Li⁺) Ions and Hydrophobic Molecules in Aqueous Solution. Journal of Chemical Theory and Computation, 2011, 7, 818-824.	5.3	8
76	The pH dependence of stability of the activation helix and the catalytic site of GART. Biophysical Chemistry, 2003, 105, 279-291.	2.8	7
77	Application of Poissonâ€"Boltzmann solvation forces to macromolecular simulations. , 1997, , 244-261.		7
78	ATP and AMP Mutually Influence Their Interaction with the ATP-binding Cassette (ABC) Adenylate Kinase Cystic Fibrosis Transmembrane Conductance Regulator (CFTR) at Separate Binding Sites. Journal of Biological Chemistry, 2013, 288, 27692-27701.	3.4	6
79	Design principles that protect the proteasome from selfâ€destruction. Protein Science, 2022, 31, 556-567.	7.6	2
80	SUBCUR: Visualization of structural differences between DNA duplexes. Journal of Molecular Graphics, 1993, 11, 211-213.	1.1	1
81	Molecular Behavior in Biological Cells: The Bacterial Cytoplasm as a Model System. , 2011, , 1-17.		0
82	Challenges to the Creation of Dynamic Structural Models of Intracellular Systems. Biophysical Journal, 2020, 118, 352a-353a.	0.5	0