Adrian H Elcock

List of Publications by Year
in descending order

82 papers	5,838 citations	87401 40 h-index	87275 74 g-index
89 all docs	89 docs citations	89 times ranked	7257 citing authors

#	Article	IF	Citations
1	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.	2.0	26
2	Design principles that protect the proteasome from selfâ€destruction. Protein Science, 2022, 31, 556-567.	3.1	2
3	Challenges to the Creation of Dynamic Structural Models of Intracellular Systems. Biophysical Journal, 2020, 118, 352a-353a.	0.2	0
4	p38Î± Mitogen-Activated Protein Kinase Is a Druggable Target in Pancreatic Adenocarcinoma. Frontiers in Oncology, 2019, 9, 1294.	1.3	20
5	Cotranslational protein assembly imposes evolutionary constraints on homomeric proteins. Nature Structural and Molecular Biology, 2018, 25, 279-288.	3.6	43
6	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.	6.5	17
7	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.	2.3	29
8	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.	2.3	22
9	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.	2.3	37
10	Features of genomic organization in a nucleotide-resolution molecular model of the Escherichia coli chromosome. Nucleic Acids Research, 2017, 45, 7541-7554.	6.5	48
11	Molecular chaperones: providing a safe place to weather a midlife protein-folding crisis. Nature Structural and Molecular Biology, 2016, 23, 621-623.	3.6	9
12	Dynamic binding of replication protein a is required for DNA repair. Nucleic Acids Research, 2016, 44, 5758-5772.	6.5	82
13	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.	1.2	28
14	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.	2.3	48
15	Residue-Specific Force Field (RSFF2) Improves the Modeling of Conformational Behavior of Peptides and Proteins. Journal of Physical Chemistry Letters, 2015, 6, 2127-2133.	2.1	26
16	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.	2.3	13
17	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.	2.3	86
18	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.	2.3	16

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19	Dynamics and Energy Contributions for Transport of Unfolded Pertactin through a Protein Nanopore. ACS Nano, 2015, 9, 9050-9061.	7.3	52
20	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.	2.3	20
21	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.	2.3	16
22	Human Heterochromatin Protein 1Î± Promotes Nucleosome Associations That Drive Chromatin Condensation. Journal of Biological Chemistry, 2014, 289, 6850-6861.	1.6	86
23	Physicochemical Properties of Cells and Their Effects on Intrinsically Disordered Proteins (IDPs). Chemical Reviews, 2014, 114, 6661-6714.	23.0	391
24	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.	2.3	120
25	Computer simulations of the bacterial cytoplasm. Biophysical Reviews, 2013, 5, 109-119.	1.5	37
26	Flexibility of the Bacterial Chaperone Trigger Factor in Microsecond-Timescale Molecular Dynamics Simulations. Biophysical Journal, 2013, 105, 732-744.	0.2	17
27	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.	2.3	36
28	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.	2.3	11
29	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.	2.3	18
30	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.	1.6	6
31	A PEGâ€Based Oligomer as a Backbone Replacement for Surfaceâ€Exposed Loops in a Protein Tertiary Structure. ChemBioChem, 2012, 13, 1107-1111.	1.3	17
32	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.	2.3	8
33	Molecular Behavior in Biological Cells: The Bacterial Cytoplasm as a Model System. , 2011, , 1-17.		0
34	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.	2.1	28
35	Models of macromolecular crowding effects and the need for quantitative comparisons with experiment. Current Opinion in Structural Biology, 2010, 20, 196-206.	2.6	257
36	Diffusion, Crowding & Protein Stability in a Dynamic Molecular Model of the Bacterial Cytoplasm. PLoS Computational Biology, 2010, 6, e1000694.	1.5	612

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37	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.	0.2	72
38	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.	2.3	25
39	Striking Effects of Hydrodynamic Interactions on the Simulated Diffusion and Folding of Proteins. Journal of Chemical Theory and Computation, 2009, 5, 242-256.	2.3	106
40	The Native 3D Organization of Bacterial Polysomes. Cell, 2009, 136, 261-271.	13.5	240
41	Native-state conformational dynamics of GART: A regulatory pH-dependent coil-helix transition examined by electrostatic calculations. Protein Science, 2008, 10, 2363-2378.	3.1	15
42	Proton transfer dynamics of GART: The pH-dependent catalytic mechanism examined by electrostatic calculations. Protein Science, 2008, 10, 2379-2392.	3.1	16
43	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.	6.6	151
44	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.	6.6	45
45	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.	6.6	97
46	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.	2.0	91
47	Structure Selection for Protein Kinase Docking and Virtual Screening:Homology Models or Crystal Structures?. Current Protein and Peptide Science, 2006, 7, 437-457.	0.7	51
48	Molecular Simulations of Cotranslational Protein Folding: Fragment Stabilities, Folding Cooperativity, and Trapping in the Ribosome. PLoS Computational Biology, 2006, 2, e98.	1.5	105
49	Rapid Computational Identification of the Targets of Protein Kinase Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 4138-4152.	2.9	50
50	Molecular Simulations Suggest Protein Salt Bridges Are Uniquely Suited to Life at High Temperatures. Journal of the American Chemical Society, 2004, 126, 2208-2214.	6.6	83
51	Molecular Simulations of Diffusion and Association in Multimacromolecular Systems. Methods in Enzymology, 2004, 383, 166-198.	0.4	29
52	The pH dependence of stability of the activation helix and the catalytic site of GART. Biophysical Chemistry, 2003, 105, 279-291.	1.5	7
53	Association Lifetimes of Hydrophobic Amino Acid Pairs Measured Directly from Molecular Dynamics Simulations. Journal of the American Chemical Society, 2003, 125, 13968-13969.	6.6	16
54	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.	3.3	58

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55	Atomistic Simulations of Competition between Substrates Binding to an Enzyme. Biophysical Journal, 2002, 82, 2326-2332.	0.2	15
56	Modeling supramolecular assemblages. Current Opinion in Structural Biology, 2002, 12, 154-160.	2.6	19
57	Progress toward virtual screening for drug side effects. Proteins: Structure, Function and Bioinformatics, 2002, 48, 664-671.	1.5	38
58	Computer Simulation of Proteinâ˜Protein Interactions. Journal of Physical Chemistry B, 2001, 105, 1504-1518.	1.2	203
59	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.	2.0	195
60	Calculation of Weak Protein-Protein Interactions: The pH Dependence of the Second Virial Coefficient. Biophysical Journal, 2001, 80, 613-625.	0.2	90
61	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.	3.3	107
62	Computer simulation of protein-protein association kinetics: acetylcholinesterase-fasciculin. Journal of Molecular Biology, 1999, 291, 149-162.	2.0	181
63	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.	2.0	90
64	Computer simulations of actin polymerization can explain the barbed-pointed end asymmetry. Journal of Molecular Biology, 1999, 294, 1181-1189.	2.0	65
65	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.	1.2	58
66	Electrostatic contributions to the stability of halophilic proteins. Journal of Molecular Biology, 1998, 280, 731-748.	2.0	202
67	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.	2.0	295
68	Continuum Solvation Model for Studying Protein Hydration Thermodynamics at High Temperatures. Journal of Physical Chemistry B, 1997, 101, 9624-9634.	1.2	49
69	Electrostatic Channeling of Substrates between Enzyme Active Sites:â€‰ Comparison of Simulation and Experiment. Biochemistry, 1997, 36, 16049-16058.	1.2	64
70	Electrostatic effects in homeodomain-DNA interactions. Journal of Molecular Biology, 1997, 267, 368-381.	2.0	52
71	Application of Poissonâ€”Boltzmann solvation forces to macromolecular simulations. , 1997, , 244-261.		7
72	Evidence for Electrostatic Channeling in a Fusion Protein of Malate Dehydrogenase and Citrate Synthaseâ€. Biochemistry, 1996, 35, 12652-12658.	1.2	70

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73	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.	6.6	64
74	Electrostatic Channeling in the Bifunctional Enzyme Dihydrofolate Reductase-thymidylate Synthase. Journal of Molecular Biology, 1996, 262, 370-374.	2.0	73
75	Mechanism of action of antifreeze polypeptide HPLC6 in solution: analysis of solvent behaviour by molecular dynamics. Chemical Physics, 1996, 204, 251-261.	0.9	16
76	Computing ionization states of proteins with a detailed charge model. Journal of Computational Chemistry, 1996, 17, 1633-1644.	1.5	139
77	Sequence Dependent Hydration of DNA: Theoretical Results. Journal of the American Chemical Society, 1995, 117, 10161-10162.	6.6	27
78	Combined Quantum and Molecular Mechanical Study of DNA Crosslinking by Nitrous Acid. Journal of the American Chemical Society, 1995, 117, 4706-4707.	6.6	43
79	SUBCUR: Visualization of structural differences between DNA duplexes. Journal of Molecular Graphics, 1993, 11, 211-213.	1.7	1
80	Relative hydration free energies of nucleic acid bases. Journal of the American Chemical Society, 1993, 115, 7930-7931.	6.6	31
81	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.	2.0	82
82	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.	2.0	17