Bruce Tidor

List of Publications by Year
in descending order

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Version: 2024-02-01

101 papers	13,801 citations	71102 41 h-index	45317 90 g-index
101 all docs	101 docs citations	101 times ranked	16113 citing authors

#	Article	IF	Citations
1	Modelling the impact of nucleolin expression level on the activity of F3 peptide-targeted pH-sensitive pegylated liposomes containing doxorubicin. Drug Delivery and Translational Research, 2022, 12, 629-646.	5.8	6
2	Entropy of Two-Molecule Correlated Translational-Rotational Motions Using the kth Nearest Neighbor Method. Journal of Chemical Theory and Computation, 2021, 17, 3039-3051.	5.3	4
3	Machine Learning Identifies Chemical Characteristics That Promote Enzyme Catalysis. Journal of the American Chemical Society, 2019, 141, 4108-4118.	13.7	57
4	Rational design of thiolase substrate specificity for metabolic engineering applications. Biotechnology and Bioengineering, 2018, 115, 2167-2182.	3.3	18
5	Intramolecular Hydrogen Bonding Restricts Gdâ€“Aquaâ€Ligand Dynamics. Angewandte Chemie - International Edition, 2017, 56, 5603-5606.	13.8	19
6	Intramolecular Hydrogen Bonding Restricts Gdâ€“Aquaâ€Ligand Dynamics. Angewandte Chemie, 2017, 129, 5695-5698.	2.0	2
7	A Fungal-Selective Cytochrome bc1 Inhibitor Impairs Virulence and Prevents the Evolution of Drug Resistance. Cell Chemical Biology, 2016, 23, 978-991.	5.2	52
8	Exploiting Temporal Collateral Sensitivity in Tumor Clonal Evolution. Cell, 2016, 165, 234-246.	28.9	111
9	Efficient Bayesian estimates for discrimination among topologically different systems biology models. Molecular BioSystems, 2015, 11, 574-584.	2.9	2
10	Molecular mechanisms and design principles for promiscuous inhibitors to avoid drug resistance: Lessons learned from HIV â€1 protease inhibition. Proteins: Structure, Function and Bioinformatics, 2015, 83, 351-372.	2.6	9
11	Multilevel modeling and value of information in clinical trial decision support. BMC Systems Biology, 2014, 8, 6.	3.0	3
12	Convergence in parameters and predictions using computational experimental design. Interface Focus, 2013, 3, 20130008.	3.0	37
13	Modeling Stem Cell Induction Processes. PLoS ONE, 2013, 8, e60240.	2.5	5
14	Testing the Substrate-Envelope Hypothesis with Designed Pairs of Compounds. ACS Chemical Biology, 2013, 8, 2433-2441.	3.4	33
15	Combined Model of Intrinsic and Extrinsic Variability for Computational Network Design with Application to Synthetic Biology. PLoS Computational Biology, 2013, 9, e1002960.	3.2	55
16	Charge Optimization Theory for Induced-Fit Ligands. Journal of Chemical Theory and Computation, 2012, 8, 4580-4592.	5.3	8
17	Efficient Calculation of Molecular Configurational Entropies Using an Information Theoretic Approximation. Journal of Physical Chemistry B, 2012, 116, 2891-2904.	2.6	81
18	Rational Approaches to Improving Selectivity in Drug Design. Journal of Medicinal Chemistry, 2012, 55, 1424-1444.	6.4	248

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19	Exploring the gap between dynamic and constraint-based models of metabolism. Metabolic Engineering, 2012, 14, 112-119.	7.0	33
20	Reply to Comment on â€œSloppy models, parameter uncertainty, and the role of experimental designâ€• Molecular BioSystems, 2011, 7, 2523.	2.9	6
21	Recycling Circuit Simulation Techniques forÂMass-Action Biochemical Kinetics. , 2011, , 115-136.		2
22	Systematic placement of structural water molecules for improved scoring of protein-ligand interactions. Protein Engineering, Design and Selection, 2011, 24, 777-789.	2.1	40
23	Delineation of Lipopolysaccharide (LPS)-binding Sites on Hemoglobin. Journal of Biological Chemistry, 2011, 286, 37793-37803.	3.4	29
24	Cellular level models as tools for cytokine design. Biotechnology Progress, 2010, 26, 919-937.	2.6	0
25	Sloppy models, parameter uncertainty, and the role of experimental design. Molecular BioSystems, 2010, 6, 1890.	2.9	114
26	Evaluating the Substrate-Envelope Hypothesis: Structural Analysis of Novel HIV-1 Protease Inhibitors Designed To Be Robust against Drug Resistance. Journal of Virology, 2010, 84, 5368-5378.	3.4	104
27	MIST: Maximum Information Spanning Trees for dimension reduction of biological data sets. Bioinformatics, 2009, 25, 1165-1172.	4.1	75
28	Accurate solution of multiâ€•region continuum biomolecule electrostatic problems using the linearized Poissonâ€“Boltzmann equation with curved boundary elements. Journal of Computational Chemistry, 2009, 30, 132-153.	3.3	80
29	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	3.3	7,077
30	Evaluation of an inverse molecular design algorithm in a model binding site. Proteins: Structure, Function and Bioinformatics, 2009, 75, 168-186.	2.6	8
31	â€œReverse-Schurâ€•Approach to Optimization with Linear PDE Constraints: Application to Biomolecule Analysis and Design. Journal of Chemical Theory and Computation, 2009, 5, 3260-3278.	5.3	8
32	A computational method for the analysis and prediction of protein:phosphopeptide-binding sites. Protein Science, 2009, 14, 131-139.	7.6	44
33	Sensitivity Analysis for Oscillating Dynamical Systems. SIAM Journal of Scientific Computing, 2009, 31, 2706-2732.	2.8	40
34	Computational design and experimental study of tighter binding peptides to an inactivated mutant of HIVâ€1 protease. Proteins: Structure, Function and Bioinformatics, 2008, 70, 678-694.	2.6	43
35	Novel Method for Probing the Specificity Binding Profile of Ligands: Applications to HIV Protease. Chemical Biology and Drug Design, 2008, 71, 387-407.	3.2	26
36	Computationally Mapping Sequence Space To Understand Evolutionary Protein Engineering. Biotechnology Progress, 2008, 24, 62-73.	2.6	7

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37	Optimal Drug Cocktail Design: Methods for Targeting Molecular Ensembles and Insights from Theoretical Model Systems. Journal of Chemical Information and Modeling, 2008, 48, 1055-1073.	5.4	33
38	HIV-1 Protease Inhibitors from Inverse Design in the Substrate Envelope Exhibit Subnanomolar Binding to Drug-Resistant Variants. Journal of the American Chemical Society, 2008, 130, 6099-6113.	13.7	105
39	Aglycosylated immunoglobulin G₁variants productively engage activating Fc receptors. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 20167-20172.	7.1	169
40	A meshless, spectrally accurate, integral equation solver for molecular surface electrostatics. ACM Journal on Emerging Technologies in Computing Systems, 2008, 4, 1-30.	2.3	4
41	Stimulus Design for Model Selection and Validation in Cell Signaling. PLoS Computational Biology, 2008, 4, e30.	3.2	71
42	Efficient optimization of electrostatic interactions between biomolecules. , 2007, , .		0
43	Numerical integration techniques for curved-element discretizations of molecule-solvent interfaces. Journal of Chemical Physics, 2007, 127, 014701.	3.0	33
44	The Per2 Negative Feedback Loop Sets the Period in the Mammalian Circadian Clock Mechanism. PLoS Computational Biology, 2007, 3, e242.	3.2	23
45	Specificity in Molecular Design:Â A Physical Framework for Probing the Determinants of Binding Specificity and Promiscuity in a Biological Environment. Journal of Physical Chemistry B, 2007, 111, 13419-13435.	2.6	28
46	Progress in computational protein design. Current Opinion in Biotechnology, 2007, 18, 305-311.	6.6	189
47	Selection of Horseradish Peroxidase Variants with Enhanced Enantioselectivity by Yeast Surface Display. Chemistry and Biology, 2007, 14, 1176-1185.	6.0	94
48	Computational design of antibody-affinity improvement beyond in vivo maturation. Nature Biotechnology, 2007, 25, 1171-1176.	17.5	310
49	FFTSVD: A Fast Multiscale Boundary-Element Method Solver Suitable for Bio-MEMS and Biomolecule Simulation. IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems, 2006, 25, 274-284.	2.7	41
50	FFTSVD: A FAST MULTISCALE BOUNDARY ELEMENT METHOD SOLVER SUITABLE FOR BIO-MEMS AND BIOMOLECULE SIMULATION. , 2006, , 143-168.		0
51	Optimal Charges in Lead Progression:Â A Structure-Based Neuraminidase Case Study. Journal of Medicinal Chemistry, 2006, 49, 2470-2477.	6.4	31
52	Rational Design of New Binding Specificity by Simultaneous Mutagenesis of Calmodulin and a Target Peptide. Biochemistry, 2006, 45, 12547-12559.	2.5	34
53	Defining Cdk5 Ligand Chemical Space with Small Molecule Inhibitors of Tau Phosphorylation. Chemistry and Biology, 2005, 12, 811-823.	6.0	63
54	Interdisciplinary research and education at the biologyâ€“engineeringâ€“computer science interface: a perspective. Drug Discovery Today, 2005, 10, 1183-1189.	6.4	20

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55	Interdisciplinary research and education at the biology-engineering-computer science interface: a perspective (reprinted article). Drug Discovery Today, 2005, 10, 1706-1712.	6.4	3
56	Design of improved protein inhibitors of HIV-1 cell entry: Optimization of electrostatic interactions at the binding interface. Proteins: Structure, Function and Bioinformatics, 2005, 60, 644-657.	2.6	34
57	Action-at-a-distance interactions enhance protein binding affinity. Protein Science, 2005, 14, 1363-1369.	7.6	33
58	X-ray structural and simulation analysis of a protein mutant: The value of a combined approach. Proteins: Structure, Function and Bioinformatics, 2004, 55, 733-742.	2.6	2
59	Computational and Experimental Probes of Symmetry Mismatches in the Arc Repressor?DNA Complex. Journal of Molecular Biology, 2004, 340, 253-253.	4.2	0
60	Computational and Experimental Probes of Symmetry Mismatches in the Arc Repressorâ€“DNA Complex. Journal of Molecular Biology, 2004, 340, 253-261.	4.2	4
61	Escherichia coli Glutaminyl-tRNA Synthetase is Electrostatically Optimized for Binding of its Cognate Substrates. Journal of Molecular Biology, 2004, 342, 435-452.	4.2	24
62	Substantial Energetic Improvement with Minimal Structural Perturbation in a High Affinity Mutant Antibody. Journal of Molecular Biology, 2004, 343, 685-701.	4.2	121
63	Evaluation of ab Initio Charge Determination Methods for Use in Continuum Solvation Calculations. Journal of Physical Chemistry B, 2003, 107, 10261-10273.	2.6	23
64	Evaluation of Electrostatic Interactions. Current Protocols in Bioinformatics, 2003, 2, Unit 8.3.	25.8	3
65	Proteomic Identification of 14-3-3Î¶ as a Mitogen-Activated Protein Kinase-Activated Protein Kinase 2 Substrate: Role in Dimer Formation and Ligand Binding. Molecular and Cellular Biology, 2003, 23, 5376-5387.	2.3	123
66	Fast methods for simulation of biomolecule electrostatics. IEEE/ACM International Conference on Computer-Aided Design, Digest of Technical Papers, 2002, , .	0.0	11
67	Rational cytokine design for increased lifetime and enhanced potency using pH-activated â€œhistidine switchingâ€• Nature Biotechnology, 2002, 20, 908-913.	17.5	150
68	Electrostatic Complementarity at Ligand Binding Sites:â€‰ Application to Chorismate Mutase. Journal of Physical Chemistry B, 2001, 105, 880-888.	2.6	72
69	Preferential Heterodimer Formation via Undercompensated Electrostatic Interactions. Journal of the American Chemical Society, 2001, 123, 1264-1265.	13.7	17
70	Optimization of binding electrostatics: Charge complementarity in the barnase-barstar protein complex. Protein Science, 2001, 10, 362-377.	7.6	119
71	Barstar is electrostatically optimized for tight binding to barnase. , 2001, 8, 73-76.		80
72	Altering dimerization specificity by changes in surface electrostatics. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 3109-3114.	7.1	21

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73	Electrostatic specificity in molecular ligand design. Journal of Chemical Physics, 2000, 112, 9120-9131.	3.0	46
74	Rational Modification of Protein Stability by the Mutation of Charged Surface Residuesâ€. Biochemistry, 2000, 39, 872-879.	2.5	197
75	Electrostatic Optimization in Ligand Complementarity and Design. Nonconvex Optimization and Its Applications, 2000, , 231-242.	0.1	1
76	Electrostatic interactions in the GCN4 leucine zipper: Substantial contributions arise from intramolecular interactions enhanced on binding. Protein Science, 1999, 8, 1381-1392.	7.6	122
77	Charge optimization leads to favorable electrostatic binding free energy. Physical Review E, 1999, 59, 5958-5961.	2.1	47
78	Long-Range Electrostatic Contributions to Proteinâ”Ligand Binding Estimated Using Protein Charge Ladders, Affinity Capillary Electrophoresis, and Continuum Electrostatic Theory. Journal of the American Chemical Society, 1999, 121, 4340-4347.	13.7	39
79	Molecular-modeling calculations of enzymatic enantioselectivity taking hydration into account. , 1998, 57, 741-745.		17
80	AmbiPack: A systematic algorithm for packing of macromolecular structures with ambiguous distance constraints. , 1998, 32, 26-42.		18
81	Computation of electrostatic complements to proteins: A case of charge stabilized binding. Protein Science, 1998, 7, 206-210.	7.6	69
82	Effects of salt bridges on protein structure and design. Protein Science, 1998, 7, 1898-1914.	7.6	83
83	Optimizing electrostatic affinity in ligandâ€“receptor binding: Theory, computation, and ligand properties. Journal of Chemical Physics, 1998, 109, 7522-7545.	3.0	75
84	Parameter Dependence in Continuum Electrostatic Calculations:â€‰ A Study Using Protein Salt Bridges. Journal of Physical Chemistry B, 1998, 102, 4404-4410.	2.6	28
85	High-Resolution Protein Design with Backbone Freedom. , 1998, 282, 1462-1467.		419
86	Optimization of electrostatic binding free energy. Journal of Chemical Physics, 1997, 106, 8681-8690.	3.0	66
87	Simulated Annealing on Coupled Free Energy Surfaces:Â Relative Solvation Energies of Small Molecules. Journal of Physical Chemistry B, 1997, 101, 9362-9374.	2.6	7
88	Computing Bounds on Free Energy Changes with One and Two Dimensional Paths. Journal of Physical Chemistry B, 1997, 101, 9402-9409.	2.6	9
89	Protein Stabilization by Removal of Unsatisfied Polar Groups:â€‰ Computational Approaches and Experimental Tests. Biochemistry, 1996, 35, 7621-7625.	2.5	89
90	Repacking protein cores with backbone freedom: structure prediction for coiled coils.. Proceedings of the National Academy of Sciences of the United States of America, 1995, 92, 8408-8412.	7.1	143

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91	Structural model for the Î²-amyloid fibril based on interstrand alignment of an antiparallel-sheet comprising a C-terminal peptide. Nature Structural and Molecular Biology, 1995, 2, 990-998.	8.2	423
92	Do salt bridges stabilize proteins? A continuum electrostatic analysis. Protein Science, 1994, 3, 211-226.	7.6	577
93	Helix-capping interaction in Î» cro protein: A free energy simulation analysis. Proteins: Structure, Function and Bioinformatics, 1994, 19, 310-323.	2.6	32
94	The Contribution of Vibrational Entropy to Molecular Association. Journal of Molecular Biology, 1994, 238, 405-414.	4.2	311
95	The contribution of cross-links to protein stability: A normal mode analysis of the configurational entropy of the native state. Proteins: Structure, Function and Bioinformatics, 1993, 15, 71-79.	2.6	72
96	Analysis of the Stability Mutant Ile96â†'Ala in Barnase, Based on Free Energy Simulations. AIP Conference Proceedings, 1991, , .	0.4	0
97	Simulation Analysis of the Stability Mutants R96H of Bacteriophage T4 Lysozyme and I96A of Barnase. Novartis Foundation Symposium, 1991, 161, 63-74.	1.1	1
98	Inelastic neutron scattering analysis of lowâ€frequency motions in proteins: Harmonic and damped harmonic models of bovine pancreatic tryspin inhibitor. Journal of Chemical Physics, 1990, 93, 2974-2991.	3.0	84
99	Transition from B to Z DNA: contribution of internal fluctuations to the configurational entropy difference. Science, 1985, 229, 571-572.	12.6	61
100	Dynamics of DNA Oligomers. Journal of Biomolecular Structure and Dynamics, 1983, 1, 231-252.	3.5	188
101	Fast methods for simulation of biomolecule electrostatics. , 0, , .		3