Bruce Tidor

List of Publications by Citations

99 papers	11,372 citations	39 h-index	101 g-index
101 ext. papers	12,676 ext. citations	8.1 avg, IF	5.7 L-index

#	Paper	IF	Citations
99	CHARMM: the biomolecular simulation program. *Journal of Computational Chemistry*, **2009**, 30, 1545-614	3.5	5515
98	Do salt bridges stabilize proteins? A continuum electrostatic analysis. *Protein Science*, **1994**, 3, 211-26	6.3	533
97	Structural model for the beta-amyloid fibril based on interstrand alignment of an antiparallel-sheet comprising a C-terminal peptide. *Nature Structural and Molecular Biology*, **1995**, 2, 990-8	17.6	398
96	High-resolution protein design with backbone freedom. *Science*, **1998**, 282, 1462-7	33.3	374
95	The contribution of vibrational entropy to molecular association. The dimerization of insulin. *Journal of Molecular Biology*, **1994**, 238, 405-14	6.5	290
94	Computational design of antibody-affinity improvement beyond in vivo maturation. *Nature Biotechnology*, **2007**, 25, 1171-6	44.5	253
93	Rational approaches to improving selectivity in drug design. *Journal of Medicinal Chemistry*, **2012**, 55, 1424-44	8.3	189
92	Rational modification of protein stability by the mutation of charged surface residues. *Biochemistry*, **2000**, 39, 872-9	3.2	188
91	Dynamics of DNA oligomers. *Journal of Biomolecular Structure and Dynamics*, **1983**, 1, 231-52	3.6	170
90	Progress in computational protein design. *Current Opinion in Biotechnology*, **2007**, 18, 305-11	11.4	165
89	Aglycosylated immunoglobulin G1 variants productively engage activating Fc receptors. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 20167-72	11.5	144
88	Rational cytokine design for increased lifetime and enhanced potency using pH-activated "histidine switching". *Nature Biotechnology*, **2002**, 20, 908-13	44.5	133
87	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, 8408-12	11.5	132
86	Electrostatic interactions in the GCN4 leucine zipper: substantial contributions arise from intramolecular interactions enhanced on binding. *Protein Science*, **1999**, 8, 1381-92	6.3	118
85	Proteomic identification of 14-3-3zeta as a mitogen-activated protein kinase-activated protein kinase 2 substrate: role in dimer formation and ligand binding. *Molecular and Cellular Biology*, **2003**, 23, 5376-87	4.8	115
84	Optimization of binding electrostatics: charge complementarity in the barnase-barstar protein complex. *Protein Science*, **2001**, 10, 362-77	6.3	113
83	Substantial energetic improvement with minimal structural perturbation in a high affinity mutant antibody. *Journal of Molecular Biology*, **2004**, 343, 685-701	6.5	105

82	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, 6099-113	16.4	95
81	Sloppy models, parameter uncertainty, and the role of experimental design. *Molecular BioSystems*, **2010**, 6, 1890-900		90
80	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, 5368-78	6.6	85
79	Protein stabilization by removal of unsatisfied polar groups: computational approaches and experimental tests. *Biochemistry*, **1996**, 35, 7621-5	3.2	84
78	Selection of horseradish peroxidase variants with enhanced enantioselectivity by yeast surface display. *Chemistry and Biology*, **2007**, 14, 1176-85		81
77	Effects of salt bridges on protein structure and design. *Protein Science*, **1998**, 7, 1898-914	6.3	79
76	Inelastic neutron scattering analysis of low-frequency motions in proteins: Harmonic and damped harmonic models of bovine pancreatic tryspin inhibitor. *Journal of Chemical Physics*, **1990**, 93, 2974-2991	3.9	78
75	Exploiting Temporal Collateral Sensitivity in Tumor Clonal Evolution. *Cell*, **2016**, 165, 234-246	56.2	77
74	Optimizing electrostatic affinity in ligand–receptor binding: Theory, computation, and ligand properties. *Journal of Chemical Physics*, **1998**, 109, 7522-7545	3.9	70
73	Accurate solution of multi-region continuum biomolecule electrostatic problems using the linearized Poisson-Boltzmann equation with curved boundary elements. *Journal of Computational Chemistry*, **2009**, 30, 132-53	3.5	69
72	Efficient calculation of molecular configurational entropies using an information theoretic approximation. *Journal of Physical Chemistry B*, **2012**, 116, 2891-904	3.4	67
71	Electrostatic Complementarity at Ligand Binding Sites: Application to Chorismate Mutase. *Journal of Physical Chemistry B*, **2001**, 105, 880-888	3.4	65
70	Computation of electrostatic complements to proteins: a case of charge stabilized binding. *Protein Science*, **1998**, 7, 206-10	6.3	64
69	Stimulus design for model selection and validation in cell signaling. *PLoS Computational Biology*, **2008**, 4, e30	5	62
68	Barstar is electrostatically optimized for tight binding to barnase. *Nature Structural Biology*, **2001**, 8, 73-6		62
67	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, 71-9	4.2	62
66	MIST: Maximum Information Spanning Trees for dimension reduction of biological data sets. *Bioinformatics*, **2009**, 25, 1165-72	7.2	60
65	Optimization of electrostatic binding free energy. *Journal of Chemical Physics*, **1997**, 106, 8681-8690	3.9	60

64	Defining Cdk5 ligand chemical space with small molecule inhibitors of tau phosphorylation. *Chemistry and Biology*, **2005**, 12, 811-23		53
63	Transition from B to Z DNA: contribution of internal fluctuations to the configurational entropy difference. *Science*, **1985**, 229, 571-2	33.3	50
62	Combined model of intrinsic and extrinsic variability for computational network design with application to synthetic biology. *PLoS Computational Biology*, **2013**, 9, e1002960	5	43
61	Charge optimization leads to favorable electrostatic binding free energy. *Physical Review E*, **1999**, 59, 5958-61	2.4	41
60	Electrostatic specificity in molecular ligand design. *Journal of Chemical Physics*, **2000**, 112, 9120-9131	3.9	39
59	Computational design and experimental study of tighter binding peptides to an inactivated mutant of HIV-1 protease. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 678-94	4.2	38
58	A computational method for the analysis and prediction of protein:phosphopeptide-binding sites. *Protein Science*, **2005**, 14, 131-9	6.3	37
57	Systematic placement of structural water molecules for improved scoring of protein-ligand interactions. *Protein Engineering, Design and Selection*, **2011**, 24, 777-89	1.9	36
56	Long-Range Electrostatic Contributions to Protein□ligand Binding Estimated Using Protein Charge Ladders, Affinity Capillary Electrophoresis, and Continuum Electrostatic Theory. *Journal of the American Chemical Society*, **1999**, 121, 4340-4347	16.4	36
55	SENSITIVITY ANALYSIS FOR OSCILLATING DYNAMICAL SYSTEMS. *SIAM Journal of Scientific Computing*, **2009**, 31, 2706-2732	2.6	32
54	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	2.5	32
53	Rational design of new binding specificity by simultaneous mutagenesis of calmodulin and a target peptide. *Biochemistry*, **2006**, 45, 12547-59	3.2	32
52	Convergence in parameters and predictions using computational experimental design. *Interface Focus*, **2013**, 3, 20130008	3.9	30
51	Action-at-a-distance interactions enhance protein binding affinity. *Protein Science*, **2005**, 14, 1363-9	6.3	29
50	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, 644-57	4.2	29
49	Parameter Dependence in Continuum Electrostatic Calculations: A Study Using Protein Salt Bridges. *Journal of Physical Chemistry B*, **1998**, 102, 4404-4410	3.4	28
48	Helix-capping interaction in lambda Cro protein: a free energy simulation analysis. *Proteins: Structure, Function and Bioinformatics*, **1994**, 19, 310-23	4.2	28
47	Machine Learning Identifies Chemical Characteristics That Promote Enzyme Catalysis. *Journal of the American Chemical Society*, **2019**, 141, 4108-4118	16.4	28

46	Testing the substrate-envelope hypothesis with designed pairs of compounds. *ACS Chemical Biology*, **2013**, 8, 2433-41	4.9	27
45	Optimal drug cocktail design: methods for targeting molecular ensembles and insights from theoretical model systems. *Journal of Chemical Information and Modeling*, **2008**, 48, 1055-73	6.1	27
44	Numerical integration techniques for curved-element discretizations of molecule-solvent interfaces. *Journal of Chemical Physics*, **2007**, 127, 014701	3.9	27
43	Optimal charges in lead progression: a structure-based neuraminidase case study. *Journal of Medicinal Chemistry*, **2006**, 49, 2470-7	8.3	27
42	Exploring the gap between dynamic and constraint-based models of metabolism. *Metabolic Engineering*, **2012**, 14, 112-9	9.7	26
41	Specificity in molecular design: a physical framework for probing the determinants of binding specificity and promiscuity in a biological environment. *Journal of Physical Chemistry B*, **2007**, 111, 13419-35	3.4	26
40	Delineation of lipopolysaccharide (LPS)-binding sites on hemoglobin: from in silico predictions to biophysical characterization. *Journal of Biological Chemistry*, **2011**, 286, 37793-803	5.4	24
39	Novel method for probing the specificity binding profile of ligands: applications to HIV protease. *Chemical Biology and Drug Design*, **2008**, 71, 387-407	2.9	22
38	Escherichia coli glutaminyl-tRNA synthetase is electrostatically optimized for binding of its cognate substrates. *Journal of Molecular Biology*, **2004**, 342, 435-52	6.5	22
37	A Fungal-Selective Cytochrome bc Inhibitor Impairs Virulence and Prevents the Evolution of Drug Resistance. *Cell Chemical Biology*, **2016**, 23, 978-991	8.2	21
36	Evaluation of ab Initio Charge Determination Methods for Use in Continuum Solvation Calculations. *Journal of Physical Chemistry B*, **2003**, 107, 10261-10273	3.4	21
35	Altering dimerization specificity by changes in surface electrostatics. *Proceedings of the National Academy of Sciences of the United States of America*, **2001**, 98, 3109-14	11.5	21
34	The Per2 negative feedback loop sets the period in the mammalian circadian clock mechanism. *PLoS Computational Biology*, **2007**, 3, e242	5	18
33	Molecular-modeling calculations of enzymatic enantioselectivity taking hydration into account. *Biotechnology and Bioengineering*, **1998**, 57, 741-5	4.9	17
32	Intramolecular Hydrogen Bonding Restricts Gd-Aqua-Ligand Dynamics. *Angewandte Chemie - International Edition*, **2017**, 56, 5603-5606	16.4	16
31	AmbiPack: a systematic algorithm for packing of macromolecular structures with ambiguous distance constraints. *Proteins: Structure, Function and Bioinformatics*, **1998**, 32, 26-42	4.2	15
30	Interdisciplinary research and education at the biology-engineering-computer science interface: a perspective. *Drug Discovery Today*, **2005**, 10, 1183-9	8.8	15
29	Preferential heterodimer formation via undercompensated electrostatic interactions. *Journal of the American Chemical Society*, **2001**, 123, 1264-5	16.4	15

28	Rational design of thiolase substrate specificity for metabolic engineering applications. *Biotechnology and Bioengineering*, **2018**, 115, 2167-2182	4.9	9
27	Evaluation of an inverse molecular design algorithm in a model binding site. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 168-86	4.2	8
26	Computing Bounds on Free Energy Changes with One and Two Dimensional Paths. *Journal of Physical Chemistry B*, **1997**, 101, 9402-9409	3.4	8
25	Simulated Annealing on Coupled Free Energy Surfaces: Relative Solvation Energies of Small Molecules. *Journal of Physical Chemistry B*, **1997**, 101, 9362-9374	3.4	7
24	Molecular mechanisms and design principles for promiscuous inhibitors to avoid drug resistance: lessons learned from HIV-1 protease inhibition. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 351-72	4.2	6
23	Charge Optimization Theory for Induced-Fit Ligands. *Journal of Chemical Theory and Computation*, **2012**, 8, 4580-4592	6.4	6
22	Reply to Comment on "Sloppy models, parameter uncertainty, and the role of experimental design". *Molecular BioSystems*, **2011**, 7, 2523-2524		6
21	A "Reverse-Schur" Approach to Optimization With Linear PDE Constraints: Application to Biomolecule Analysis and Design. *Journal of Chemical Theory and Computation*, **2009**, 5, 3260-3278	6.4	6
20	Computationally mapping sequence space to understand evolutionary protein engineering. *Biotechnology Progress*, **2008**, 24, 62-73	2.8	6
19	Fast methods for simulation of biomolecule electrostatics. *IEEE/ACM International Conference on Computer-Aided Design, Digest of Technical Papers*, **2002**,		5
18	Modeling stem cell induction processes. *PLoS ONE*, **2013**, 8, e60240	3.7	4
17	Computational and experimental probes of symmetry mismatches in the Arc repressor-DNA complex. *Journal of Molecular Biology*, **2004**, 340, 253-61	6.5	4
16	A meshless, spectrally accurate, integral equation solver for molecular surface electrostatics. *ACM Journal on Emerging Technologies in Computing Systems*, **2008**, 4, 1-30	1.7	3
15	Evaluation of electrostatic interactions. *Current Protocols in Bioinformatics*, **2003**, Chapter 8, Unit 8.3	24.2	3
14	Interdisciplinary research and education at the biology-engineering-computer science interface: a perspective (reprinted article). *Drug Discovery Today*, **2005**, 10, 1706-1712	8.8	3
13	Fast methods for simulation of biomolecule electrostatics		3
12	Intramolecular Hydrogen Bonding Restricts Gd□Aqua-Ligand Dynamics. *Angewandte Chemie*, **2017**, 129, 5695-5698	3.6	2
11	Efficient Bayesian estimates for discrimination among topologically different systems biology models. *Molecular BioSystems*, **2015**, 11, 574-84		2

10	Recycling Circuit Simulation Techniques for Mass-Action Biochemical Kinetics **2011**, 115-136		2
9	X-ray structural and simulation analysis of a protein mutant: the value of a combined approach. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 733-42	4.2	2
8	Entropy of Two-Molecule Correlated Translational-Rotational Motions Using the th Nearest Neighbor Method. *Journal of Chemical Theory and Computation*, **2021**, 17, 3039-3051	6.4	2
7	Multilevel modeling and value of information in clinical trial decision support. *BMC Systems Biology*, **2014**, 8, 6	3.5	1
6	Electrostatic Optimization in Ligand Complementarity and Design. *Nonconvex Optimization and Its Applications*, **2000**, 231-242		1
5	Simulation analysis of the stability mutants R96H of bacteriophage T4 lysozyme and I96A of barnase. *Novartis Foundation Symposium*, **1991**, 161, 63-74		0
4	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*, **2021**, 1	6.2	0
3	Cellular level models as tools for cytokine design. *Biotechnology Progress*, **2010**, 26, 919-37	2.8	
2	FFTSVD: A FAST MULTISCALE BOUNDARY ELEMENT METHOD SOLVER SUITABLE FOR BIO-MEMS AND BIOMOLECULE SIMULATION **2006**, 143-168		
1	Computational and Experimental Probes of Symmetry Mismatches in the Arc Repressor?DNA Complex. *Journal of Molecular Biology*, **2004**, 340, 253-253	6.5	