

Bruce Tidor

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/9577330/publications.pdf>

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	CHARMM: The biomolecular simulation program. <i>Journal of Computational Chemistry</i> , 2009, 30, 1545-1614.	3.3	7,077
2	Do salt bridges stabilize proteins? A continuum electrostatic analysis. <i>Protein Science</i> , 1994, 3, 211-226.	7.6	577
3	Structural model for the β^2 -amyloid fibril based on interstrand alignment of an antiparallel-sheet comprising a C-terminal peptide. <i>Nature Structural and Molecular Biology</i> , 1995, 2, 990-998.	8.2	423
4	High-Resolution Protein Design with Backbone Freedom. , 1998, 282, 1462-1467.		419
5	The Contribution of Vibrational Entropy to Molecular Association. <i>Journal of Molecular Biology</i> , 1994, 238, 405-414.	4.2	311
6	Computational design of antibody-affinity improvement beyond in vivo maturation. <i>Nature Biotechnology</i> , 2007, 25, 1171-1176.	17.5	310
7	Rational Approaches to Improving Selectivity in Drug Design. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 1424-1444.	6.4	248
8	Rational Modification of Protein Stability by the Mutation of Charged Surface Residues. <i>Biochemistry</i> , 2000, 39, 872-879.	2.5	197
9	Progress in computational protein design. <i>Current Opinion in Biotechnology</i> , 2007, 18, 305-311.	6.6	189
10	Dynamics of DNA Oligomers. <i>Journal of Biomolecular Structure and Dynamics</i> , 1983, 1, 231-252.	3.5	188
11	Aglycosylated immunoglobulin G ₁ variants productively engage activating Fc receptors. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 20167-20172.	7.1	169
12	Rational cytokine design for increased lifetime and enhanced potency using pH-activated histidine switching. <i>Nature Biotechnology</i> , 2002, 20, 908-913.	17.5	150
13	Repacking protein cores with backbone freedom: structure prediction for coiled coils. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1995, 92, 8408-8412.	7.1	143
14	Proteomic Identification of 14-3-3 η as a Mitogen-Activated Protein Kinase-Activated Protein Kinase 2 Substrate: Role in Dimer Formation and Ligand Binding. <i>Molecular and Cellular Biology</i> , 2003, 23, 5376-5387.	2.3	123
15	Electrostatic interactions in the GCN4 leucine zipper: Substantial contributions arise from intramolecular interactions enhanced on binding. <i>Protein Science</i> , 1999, 8, 1381-1392.	7.6	122
16	Substantial Energetic Improvement with Minimal Structural Perturbation in a High Affinity Mutant Antibody. <i>Journal of Molecular Biology</i> , 2004, 343, 685-701.	4.2	121
17	Optimization of binding electrostatics: Charge complementarity in the barnase-barstar protein complex. <i>Protein Science</i> , 2001, 10, 362-377.	7.6	119
18	Sloppy models, parameter uncertainty, and the role of experimental design. <i>Molecular BioSystems</i> , 2010, 6, 1890.	2.9	114

#	ARTICLE	IF	CITATIONS
19	Exploiting Temporal Collateral Sensitivity in Tumor Clonal Evolution. <i>Cell</i> , 2016, 165, 234-246.	28.9	111
20	HIV-1 Protease Inhibitors from Inverse Design in the Substrate Envelope Exhibit Subnanomolar Binding to Drug-Resistant Variants. <i>Journal of the American Chemical Society</i> , 2008, 130, 6099-6113.	13.7	105
21	Evaluating the Substrate-Envelope Hypothesis: Structural Analysis of Novel HIV-1 Protease Inhibitors Designed To Be Robust against Drug Resistance. <i>Journal of Virology</i> , 2010, 84, 5368-5378.	3.4	104
22	Selection of Horseradish Peroxidase Variants with Enhanced Enantioselectivity by Yeast Surface Display. <i>Chemistry and Biology</i> , 2007, 14, 1176-1185.	6.0	94
23	Protein Stabilization by Removal of Unsatisfied Polar Groups: Computational Approaches and Experimental Tests. <i>Biochemistry</i> , 1996, 35, 7621-7625.	2.5	89
24	Inelastic neutron scattering analysis of low-frequency motions in proteins: Harmonic and damped harmonic models of bovine pancreatic trypsin inhibitor. <i>Journal of Chemical Physics</i> , 1990, 93, 2974-2991.	3.0	84
25	Effects of salt bridges on protein structure and design. <i>Protein Science</i> , 1998, 7, 1898-1914.	7.6	83
26	Efficient Calculation of Molecular Configurational Entropies Using an Information Theoretic Approximation. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2891-2904.	2.6	81
27	Barstar is electrostatically optimized for tight binding to barnase. , 2001, 8, 73-76.		80
28	Accurate solution of multi-region continuum biomolecule electrostatic problems using the linearized Poisson-Boltzmann equation with curved boundary elements. <i>Journal of Computational Chemistry</i> , 2009, 30, 132-153.	3.3	80
29	Optimizing electrostatic affinity in ligand-receptor binding: Theory, computation, and ligand properties. <i>Journal of Chemical Physics</i> , 1998, 109, 7522-7545.	3.0	75
30	MIST: Maximum Information Spanning Trees for dimension reduction of biological data sets. <i>Bioinformatics</i> , 2009, 25, 1165-1172.	4.1	75
31	The contribution of cross-links to protein stability: A normal mode analysis of the configurational entropy of the native state. <i>Proteins: Structure, Function and Bioinformatics</i> , 1993, 15, 71-79.	2.6	72
32	Electrostatic Complementarity at Ligand Binding Sites: Application to Chorismate Mutase. <i>Journal of Physical Chemistry B</i> , 2001, 105, 880-888.	2.6	72
33	Stimulus Design for Model Selection and Validation in Cell Signaling. <i>PLoS Computational Biology</i> , 2008, 4, e30.	3.2	71
34	Computation of electrostatic complements to proteins: A case of charge stabilized binding. <i>Protein Science</i> , 1998, 7, 206-210.	7.6	69
35	Optimization of electrostatic binding free energy. <i>Journal of Chemical Physics</i> , 1997, 106, 8681-8690.	3.0	66
36	Defining Cdk5 Ligand Chemical Space with Small Molecule Inhibitors of Tau Phosphorylation. <i>Chemistry and Biology</i> , 2005, 12, 811-823.	6.0	63

#	ARTICLE	IF	CITATIONS
37	Transition from B to Z DNA: contribution of internal fluctuations to the configurational entropy difference. <i>Science</i> , 1985, 229, 571-572.	12.6	61
38	Machine Learning Identifies Chemical Characteristics That Promote Enzyme Catalysis. <i>Journal of the American Chemical Society</i> , 2019, 141, 4108-4118.	13.7	57
39	Combined Model of Intrinsic and Extrinsic Variability for Computational Network Design with Application to Synthetic Biology. <i>PLoS Computational Biology</i> , 2013, 9, e1002960.	3.2	55
40	A Fungal-Selective Cytochrome bc1 Inhibitor Impairs Virulence and Prevents the Evolution of Drug Resistance. <i>Cell Chemical Biology</i> , 2016, 23, 978-991.	5.2	52
41	Charge optimization leads to favorable electrostatic binding free energy. <i>Physical Review E</i> , 1999, 59, 5958-5961.	2.1	47
42	Electrostatic specificity in molecular ligand design. <i>Journal of Chemical Physics</i> , 2000, 112, 9120-9131.	3.0	46
43	A computational method for the analysis and prediction of protein:phosphopeptide-binding sites. <i>Protein Science</i> , 2009, 14, 131-139.	7.6	44
44	Computational design and experimental study of tighter binding peptides to an inactivated mutant of HIV-1 protease. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 678-694.	2.6	43
45	FFTSVD: A Fast Multiscale Boundary-Element Method Solver Suitable for Bio-MEMS and Biomolecule Simulation. <i>IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems</i> , 2006, 25, 274-284.	2.7	41
46	Sensitivity Analysis for Oscillating Dynamical Systems. <i>SIAM Journal of Scientific Computing</i> , 2009, 31, 2706-2732.	2.8	40
47	Systematic placement of structural water molecules for improved scoring of protein-ligand interactions. <i>Protein Engineering, Design and Selection</i> , 2011, 24, 777-789.	2.1	40
48	Long-Range Electrostatic Contributions to Protein-Ligand Binding Estimated Using Protein Charge Ladders, Affinity Capillary Electrophoresis, and Continuum Electrostatic Theory. <i>Journal of the American Chemical Society</i> , 1999, 121, 4340-4347.	13.7	39
49	Convergence in parameters and predictions using computational experimental design. <i>Interface Focus</i> , 2013, 3, 20130008.	3.0	37
50	Design of improved protein inhibitors of HIV-1 cell entry: Optimization of electrostatic interactions at the binding interface. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 60, 644-657.	2.6	34
51	Rational Design of New Binding Specificity by Simultaneous Mutagenesis of Calmodulin and a Target Peptide. <i>Biochemistry</i> , 2006, 45, 12547-12559.	2.5	34
52	Action-at-a-distance interactions enhance protein binding affinity. <i>Protein Science</i> , 2005, 14, 1363-1369.	7.6	33
53	Numerical integration techniques for curved-element discretizations of molecule-solvent interfaces. <i>Journal of Chemical Physics</i> , 2007, 127, 014701.	3.0	33
54	Optimal Drug Cocktail Design: Methods for Targeting Molecular Ensembles and Insights from Theoretical Model Systems. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1055-1073.	5.4	33

#	ARTICLE	IF	CITATIONS
55	Exploring the gap between dynamic and constraint-based models of metabolism. <i>Metabolic Engineering</i> , 2012, 14, 112-119.	7.0	33
56	Testing the Substrate-Envelope Hypothesis with Designed Pairs of Compounds. <i>ACS Chemical Biology</i> , 2013, 8, 2433-2441.	3.4	33
57	Helix-capping interaction in λ cro protein: A free energy simulation analysis. <i>Proteins: Structure, Function and Bioinformatics</i> , 1994, 19, 310-323.	2.6	32
58	Optimal Charges in Lead Progression: A Structure-Based Neuraminidase Case Study. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 2470-2477.	6.4	31
59	Delineation of Lipopolysaccharide (LPS)-binding Sites on Hemoglobin. <i>Journal of Biological Chemistry</i> , 2011, 286, 37793-37803.	3.4	29
60	Parameter Dependence in Continuum Electrostatic Calculations: A Study Using Protein Salt Bridges. <i>Journal of Physical Chemistry B</i> , 1998, 102, 4404-4410.	2.6	28
61	Specificity in Molecular Design: A Physical Framework for Probing the Determinants of Binding Specificity and Promiscuity in a Biological Environment. <i>Journal of Physical Chemistry B</i> , 2007, 111, 13419-13435.	2.6	28
62	Novel Method for Probing the Specificity Binding Profile of Ligands: Applications to HIV Protease. <i>Chemical Biology and Drug Design</i> , 2008, 71, 387-407.	3.2	26
63	<i>Escherichia coli</i> Glutamyl-tRNA Synthetase is Electrostatically Optimized for Binding of its Cognate Substrates. <i>Journal of Molecular Biology</i> , 2004, 342, 435-452.	4.2	24
64	Evaluation of ab Initio Charge Determination Methods for Use in Continuum Solvation Calculations. <i>Journal of Physical Chemistry B</i> , 2003, 107, 10261-10273.	2.6	23
65	The Per2 Negative Feedback Loop Sets the Period in the Mammalian Circadian Clock Mechanism. <i>PLoS Computational Biology</i> , 2007, 3, e242.	3.2	23
66	Altering dimerization specificity by changes in surface electrostatics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2001, 98, 3109-3114.	7.1	21
67	Interdisciplinary research and education at the biology-engineering-computer science interface: a perspective. <i>Drug Discovery Today</i> , 2005, 10, 1183-1189.	6.4	20
68	Intramolecular Hydrogen Bonding Restricts G-protein Ligand Dynamics. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 5603-5606.	13.8	19
69	AmbiPack: A systematic algorithm for packing of macromolecular structures with ambiguous distance constraints. <i>Journal of Molecular Biology</i> , 1998, 32, 26-42.		18
70	Rational design of thiolase substrate specificity for metabolic engineering applications. <i>Biotechnology and Bioengineering</i> , 2018, 115, 2167-2182.	3.3	18
71	Molecular-modeling calculations of enzymatic enantioselectivity taking hydration into account. <i>Journal of Physical Chemistry B</i> , 1998, 57, 741-745.		17
72	Preferential Heterodimer Formation via Undercompensated Electrostatic Interactions. <i>Journal of the American Chemical Society</i> , 2001, 123, 1264-1265.	13.7	17

#	ARTICLE	IF	CITATIONS
73	Fast methods for simulation of biomolecule electrostatics. IEEE/ACM International Conference on Computer-Aided Design, Digest of Technical Papers, 2002, , .	0.0	11
74	Computing Bounds on Free Energy Changes with One and Two Dimensional Paths. Journal of Physical Chemistry B, 1997, 101, 9402-9409.	2.6	9
75	Molecular mechanisms and design principles for promiscuous inhibitors to avoid drug resistance: Lessons learned from HIV α 1 protease inhibition. Proteins: Structure, Function and Bioinformatics, 2015, 83, 351-372.	2.6	9
76	Evaluation of an inverse molecular design algorithm in a model binding site. Proteins: Structure, Function and Bioinformatics, 2009, 75, 168-186.	2.6	8
77	α Reverse-Schur α 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
78	Charge Optimization Theory for Induced-Fit Ligands. Journal of Chemical Theory and Computation, 2012, 8, 4580-4592.	5.3	8
79	Simulated Annealing on Coupled Free Energy Surfaces: \hat{A} Relative Solvation Energies of Small Molecules. Journal of Physical Chemistry B, 1997, 101, 9362-9374.	2.6	7
80	Computationally Mapping Sequence Space To Understand Evolutionary Protein Engineering. Biotechnology Progress, 2008, 24, 62-73.	2.6	7
81	Reply to Comment on α Sloppy models, parameter uncertainty, and the role of experimental design α . Molecular BioSystems, 2011, 7, 2523.	2.9	6
82	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
83	Modeling Stem Cell Induction Processes. PLoS ONE, 2013, 8, e60240.	2.5	5
84	Computational and Experimental Probes of Symmetry Mismatches in the Arc Repressor α DNA Complex. Journal of Molecular Biology, 2004, 340, 253-261.	4.2	4
85	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
86	Entropy of Two-Molecule Correlated Translational-Rotational Motions Using the $\langle i \rangle k \langle i \rangle$ th Nearest Neighbor Method. Journal of Chemical Theory and Computation, 2021, 17, 3039-3051.	5.3	4
87	Fast methods for simulation of biomolecule electrostatics. , 0, , .		3
88	Evaluation of Electrostatic Interactions. Current Protocols in Bioinformatics, 2003, 2, Unit 8.3.	25.8	3
89	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
90	Multilevel modeling and value of information in clinical trial decision support. BMC Systems Biology, 2014, 8, 6.	3.0	3

#	ARTICLE	IF	CITATIONS
91	X-ray structural and simulation analysis of a protein mutant: The value of a combined approach. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 55, 733-742.	2.6	2
92	Recycling Circuit Simulation Techniques for Mass-Action Biochemical Kinetics. , 2011, , 115-136.		2
93	Efficient Bayesian estimates for discrimination among topologically different systems biology models. <i>Molecular BioSystems</i> , 2015, 11, 574-584.	2.9	2
94	Intramolecular Hydrogen Bonding Restricts Gd ³⁺ Ligand Dynamics. <i>Angewandte Chemie</i> , 2017, 129, 5695-5698.	2.0	2
95	Electrostatic Optimization in Ligand Complementarity and Design. <i>Nonconvex Optimization and Its Applications</i> , 2000, , 231-242.	0.1	1
96	Simulation Analysis of the Stability Mutants R96H of Bacteriophage T4 Lysozyme and I96A of Barnase. <i>Novartis Foundation Symposium</i> , 1991, 161, 63-74.	1.1	1
97	Analysis of the Stability Mutant Ile96 [†] Ala in Barnase, Based on Free Energy Simulations. <i>AIP Conference Proceedings</i> , 1991, , .	0.4	0
98	Computational and Experimental Probes of Symmetry Mismatches in the Arc Repressor?DNA Complex. <i>Journal of Molecular Biology</i> , 2004, 340, 253-253.	4.2	0
99	FFTSVD: A FAST MULTISCALE BOUNDARY ELEMENT METHOD SOLVER SUITABLE FOR BIO-MEMS AND BIOMOLECULE SIMULATION. , 2006, , 143-168.		0
100	Efficient optimization of electrostatic interactions between biomolecules. , 2007, , .		0
101	Cellular level models as tools for cytokine design. <i>Biotechnology Progress</i> , 2010, 26, 919-937.	2.6	0