

Yuk Y Sham

List of Publications by Year in descending order

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77
papers

3,629
citations

147566

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84
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docs citations

84
times ranked

4556
citing authors

#	ARTICLE	IF	CITATIONS
1	Consistent Calculations of pKa's of Ionizable Residues in Proteins: Semi-microscopic and Microscopic Approaches. <i>Journal of Physical Chemistry B</i> , 1997, 101, 4458-4472.	1.2	357
2	Blue Gene: A vision for protein science using a petaflop supercomputer. <i>IBM Systems Journal</i> , 2001, 40, 310-327.	3.1	211
3	The Effect of Protein Relaxation on Charge-Charge Interactions and Dielectric Constants of Proteins. <i>Biophysical Journal</i> , 1998, 74, 1744-1753.	0.2	207
4	Examining methods for calculations of binding free energies: LRA, LIE, PDL-D-LRA, and PDL-D/S-LRA calculations of ligands binding to an HIV protease. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 39, 393-407.	1.5	202
5	Structured disorder and conformational selection. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 44, 418-427.	1.5	184
6	How important are entropic contributions to enzyme catalysis?. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2000, 97, 11899-11904.	3.3	178
7	Calculations of Activation Entropies of Chemical Reactions in Solution. <i>Journal of Physical Chemistry B</i> , 2000, 104, 4578-4584.	1.2	166
8	Rapid Identification of Keap1-Nrf2 Small-Molecule Inhibitors through Structure-Based Virtual Screening and Hit-Based Substructure Search. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 1121-1126.	2.9	127
9	Direct Inhibition of Insulin-Like Growth Factor-I Receptor Kinase Activity by (âˆ“)âˆ“) Epigallocatechin-3-Gallate Regulates Cell Transformation. <i>Cancer Epidemiology Biomarkers and Prevention</i> , 2007, 16, 598-605.	1.1	121
10	A Universal Method for the Preparation of Covalent Protein-DNA Conjugates for Use in Creating Protein Nanostructures. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 8819-8822.	7.2	103
11	Platelet Factor 4 and Interleukin-8 CXC Chemokine Heterodimer Formation Modulates Function at the Quaternary Structural Level. <i>Journal of Biological Chemistry</i> , 2005, 280, 4948-4958.	1.6	86
12	Simulating proton translocations in proteins: Probing proton transfer pathways in the Rhodospirillum rubrum reaction center. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 36, 484-500.	1.5	81
13	The design, synthesis and biological evaluations of C-6 or C-7 substituted 2-hydroxyisoquinoline-1,3-diones as inhibitors of hepatitis C virus. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 467-479.	1.4	66
14	CXC and CC Chemokines Form Mixed Heterodimers. <i>Journal of Biological Chemistry</i> , 2008, 283, 24155-24166.	1.6	65
15	Triazole-Linked Inhibitors of Inosine Monophosphate Dehydrogenase from Human and <i>Mycobacterium tuberculosis</i> . <i>Journal of Medicinal Chemistry</i> , 2010, 53, 4768-4778.	2.9	65
16	Blue Matter, an application framework for molecular simulation on Blue Gene. <i>Journal of Parallel and Distributed Computing</i> , 2003, 63, 759-773.	2.7	62
17	N-3 Hydroxylation of Pyrimidine-2,4-diones Yields Dual Inhibitors of HIV Reverse Transcriptase and Integrase. <i>ACS Medicinal Chemistry Letters</i> , 2011, 2, 63-67.	1.3	61
18	The surface constraint all atom model provides size independent results in calculations of hydration free energies. <i>Journal of Chemical Physics</i> , 1998, 109, 7940-7944.	1.2	60

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19	5-Arylidene-thiothiazolidinones as Inhibitors of Tyrosyl-DNA Phosphodiesterase I. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 8671-8684.	2.9	56
20	3-Hydroxypyrimidine-2,4-diones as an Inhibitor Scaffold of HIV Integrase. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 2282-2292.	2.9	54
21	Inhibition of Inflammatory and Neuropathic Pain by Targeting a Mu Opioid Receptor/Chemokine Receptor5 Heteromer (MOR-CCR5). <i>Journal of Medicinal Chemistry</i> , 2015, 58, 8647-8657.	2.9	53
22	A critical role for the loop region of the basic helix-loop-helix/leucine zipper protein Mlx in DNA binding and glucose-regulated transcription. <i>Nucleic Acids Research</i> , 2006, 35, 35-44.	6.5	51
23	Homology Modeling and Molecular Dynamics Simulations of the Mu Opioid Receptor in a Membrane-Aqueous System. <i>ChemBioChem</i> , 2005, 6, 853-859.	1.3	46
24	Development of selective inhibitors for anti-apoptotic Bcl-2 proteins from BHI-1. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 2167-2176.	1.4	44
25	Muscle membrane integrity in Duchenne muscular dystrophy: recent advances in copolymer-based muscle membrane stabilizers. <i>Skeletal Muscle</i> , 2018, 8, 31.	1.9	41
26	Dual inhibitors of inosine monophosphate dehydrogenase and histone deacetylase based on a cinnamic hydroxamic acid core structure. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 5950-5964.	1.4	40
27	Thermal unfolding molecular dynamics simulation of Escherichia coli dihydrofolate reductase: Thermal stability of protein domains and unfolding pathway. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002, 46, 308-320.	1.5	39
28	6-Benzoyl-3-hydroxypyrimidine-2,4-diones as dual inhibitors of HIV reverse transcriptase and integrase. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2011, 21, 2400-2402.	1.0	37
29	An Indole-Chalcone Inhibits Multidrug-Resistant Cancer Cell Growth by Targeting Microtubules. <i>Molecular Pharmaceutics</i> , 2018, 15, 3892-3900.	2.3	36
30	Protein Folding and Function: The N-Terminal Fragment in Adenylate Kinase. <i>Biophysical Journal</i> , 2001, 80, 2439-2454.	0.2	35
31	Design, asymmetric synthesis, and evaluation of pseudosymmetric sulfoximine inhibitors against HIV-1 protease. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 2037-2048.	1.4	35
32	Bypass of DNA-Protein Cross-links Conjugated to the 7-Deazaguanine Position of DNA by Translesion Synthesis Polymerases. <i>Journal of Biological Chemistry</i> , 2016, 291, 23589-23603.	1.6	33
33	Design and synthesis of sulfoximine based inhibitors for HIV-1 protease. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2008, 18, 5406-5410.	1.0	31
34	Shared Catalysis in Virus Entry and Bacterial Cell Wall Depolymerization. <i>Journal of Molecular Biology</i> , 2009, 387, 607-618.	2.0	28
35	Scaffold rearrangement of dihydroxypyrimidine inhibitors of HIV integrase: Docking model revisited. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 3275-3279.	1.0	28
36	pH-Dependent Transport of Pemetrexed by Breast Cancer Resistance Protein. <i>Drug Metabolism and Disposition</i> , 2011, 39, 1478-1485.	1.7	28

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37	Chemical End Group Modified Diblock Copolymers Elucidate Anchor and Chain Mechanism of Membrane Stabilization. <i>Molecular Pharmaceutics</i> , 2017, 14, 2333-2339.	2.3	28
38	All-Atom Molecular Dynamics-Based Analysis of Membrane-Stabilizing Copolymer Interactions with Lipid Bilayers Probed under Constant Surface Tensions. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10657-10664.	1.2	27
39	CD200 Checkpoint Reversal: A Novel Approach to Immunotherapy. <i>Clinical Cancer Research</i> , 2020, 26, 232-241.	3.2	25
40	Maintenance DNA Methyltransferase Activity in the Presence of Oxidized Forms of 5-Methylcytosine: Structural Basis for Ten Eleven Translocation-Mediated DNA Demethylation. <i>Biochemistry</i> , 2018, 57, 6061-6069.	1.2	23
41	Discovery of 1-hydroxypyridine-2-thiones as selective histone deacetylase inhibitors and their potential application for treating leukemia. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015, 25, 4320-4324.	1.0	22
42	Selective inhibition of nicotinamide adenine dinucleotide kinases by dinucleoside disulfide mimics of nicotinamide adenine dinucleotide analogues. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 5656-5664.	1.4	21
43	Aptamer adaptive binding assessed by stilbene photoisomerization towards regenerating aptasensors. <i>Sensors and Actuators B: Chemical</i> , 2018, 257, 245-255.	4.0	21
44	Structure and Stability of Human Telomeric G-Quadruplex with Preclinical 9-Amino Acridines. <i>PLoS ONE</i> , 2013, 8, e57701.	1.1	21
45	Pathogenic peptide deviations support a model of adaptive evolution of chordate cardiac performance by troponin mutations. <i>Physiological Genomics</i> , 2010, 42, 287-299.	1.0	20
46	The Stories Tryptophans Tell: Exploring Protein Dynamics of Heptosyltransferase I from <i>Escherichia coli</i> . <i>Biochemistry</i> , 2017, 56, 886-895.	1.2	20
47	Peptide/Receptor Co-evolution Explains the Lipolytic Function of the Neuropeptide TLQP-21. <i>Cell Reports</i> , 2019, 28, 2567-2580.e6.	2.9	20
48	Molecular dynamics simulation of <i>Escherichia coli</i> dihydrofolate reductase and its protein fragments: Relative stabilities in experiment and simulations. <i>Protein Science</i> , 2001, 10, 135-148.	3.1	19
49	Amiodarone Analog-Dependent Effects on CYP2C9-Mediated Metabolism and Kinetic Profiles. <i>Drug Metabolism and Disposition</i> , 2006, 34, 1688-1696.	1.7	18
50	Mosquito salivary allergen Aed a 3: cloning, comprehensive molecular analysis, and clinical evaluation. <i>Allergy: European Journal of Allergy and Clinical Immunology</i> , 2016, 71, 621-628.	2.7	18
51	Discovery of 1-Hydroxypyridine-2-thione-6-carboxylic Acid as a First-Class Low-Cytotoxic, Nanomolar Metallo- β -Lactamase Inhibitor. <i>ChemMedChem</i> , 2017, 12, 845-849.	1.6	18
52	A continuous fluorescence displacement assay for BioA: An enzyme involved in biotin biosynthesis. <i>Analytical Biochemistry</i> , 2011, 416, 27-38.	1.1	17
53	Impact of the C-Terminal Loop of Histidine Triad Nucleotide Binding Protein1 (Hint1) on Substrate Specificity. <i>Biochemistry</i> , 2007, 46, 13074-13079.	1.2	15
54	Temperature dependent near UV molar absorptivities of several small aldehydes in aqueous solution. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1995, 51, 247-251.	2.0	12

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55	pH-Responsive Titratable Inotropic Performance of Histidine-Modified Cardiac Troponin I. <i>Biophysical Journal</i> , 2012, 102, 1570-1579.	0.2	12
56	Cell permeable vanX inhibitors as vancomycin re-sensitizing agents. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2014, 24, 2535-2538.	1.0	11
57	Molecular Determinants of Cardiac Myocyte Performance as Conferred by Isoform-Specific TnI Residues. <i>Biophysical Journal</i> , 2014, 106, 2105-2114.	0.2	11
58	Opposites Attract: <i>Escherichia coli</i> Heptosyltransferase I Conformational Changes Induced by Interactions between the Substrate and Positively Charged Residues. <i>Biochemistry</i> , 2020, 59, 3135-3147.	1.2	11
59	A novel drug discovery strategy: Mechanistic investigation of an enantiomeric antitumor agent targeting dual p53 and NF- κ B pathways. <i>Oncotarget</i> , 2014, 5, 10830-10839.	0.8	11
60	Can 5-methylcytosine analogues with extended alkyl side chains guide DNA methylation?. <i>Chemical Communications</i> , 2018, 54, 1061-1064.	2.2	10
61	Conserved Conformational Hierarchy across Functionally Divergent Glycosyltransferases of the GT-B Structural Superfamily as Determined from Microsecond Molecular Dynamics. <i>International Journal of Molecular Sciences</i> , 2021, 22, 4619.	1.8	10
62	NAD ⁺ enhances ribitol and ribose rescue of α -dystroglycan functional glycosylation in human FKRP-mutant myotubes. <i>ELife</i> , 2021, 10, .	2.8	9
63	Ligand-Induced Conformational and Dynamical Changes in a GT-B Glycosyltransferase: Molecular Dynamics Simulations of Heptosyltransferase I Complexes. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 324-339.	2.5	8
64	TnI Structural Interface with the N-Terminal Lobe of α TnC as a Determinant of Cardiac Contractility. <i>Biophysical Journal</i> , 2018, 114, 1646-1656.	0.2	6
65	CD200 Immune-Checkpoint Peptide Elicits an Anti-glioma Response Through the DAP10 Signaling Pathway. <i>Neurotherapeutics</i> , 2021, 18, 1980-1994.	2.1	6
66	Discovery of first-in-class nanomolar inhibitors of heptosyltransferase I reveals a new aminoglycoside target and potential alternative mechanism of action. <i>Scientific Reports</i> , 2022, 12, 7302.	1.6	5
67	Mutations in the Amino Terminus of Herpes Simplex Virus Type 1 gL Can Reduce Cell-Cell Fusion without Affecting gH/gL Trafficking. <i>Journal of Virology</i> , 2014, 88, 739-744.	1.5	4
68	Modeling and Simulation of hGAT1: A Mechanistic Investigation of the GABA Transport Process. <i>Computational and Structural Biotechnology Journal</i> , 2019, 17, 61-69.	1.9	4
69	Examining methods for calculations of binding free energies: LRA, LIE, PDL-D-LRA, and PDL-D/S-LRA calculations of ligands binding to an HIV protease. , 2000, 39, 393.		4
70	Facile and Adaptable Synthesis of a Prazosin Analogue Library: Bringing Medicinal Chemistry into the Undergraduate Curriculum. <i>Journal of Chemical Education</i> , 2022, 99, 1428-1434.	1.1	4
71	Fragment-based screening and hit-based substructure search: Rapid discovery of 8-hydroxyquinoline-7-carboxylic acid as a low-cytotoxic, nanomolar metallo- β -lactamase inhibitor. <i>Chemical Biology and Drug Design</i> , 2021, 98, 481-492.	1.5	3
72	The molecular identity of the TLQP-21 peptide receptor. <i>Cellular and Molecular Life Sciences</i> , 2021, 78, 7133-7144.	2.4	3

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73	Case study: an environment for understanding protein simulations using game graphics. , 0, , .		1
74	Simulating proton translocations in proteins: Probing proton transfer pathways in the Rhodobacter sphaeroides reaction center. , 1999, 36, 484.		1
75	Computational Studies of a pH Responsive Histidine-Modified Cardiac Troponin I. Biophysical Journal, 2012, 102, 736a.	0.2	0
76	Molecular Mechanisms of A164H cTnl. Biophysical Journal, 2012, 102, 560a-561a.	0.2	0
77	Borrowing from the Platypus: Proline Substitution in Cardiac Troponin I. Biophysical Journal, 2015, 108, 447a.	0.2	0