Yuk Y Sham

List of Publications by Year
in descending order

77 papers	3,629 citations	147566 31 h-index	133063 59 g-index
84 all docs	84 docs citations	84 times ranked	4556 citing authors

#	Article	IF	Citations
1	Facile and Adaptable Synthesis of a Prazosin Analogue Library: Bringing Medicinal Chemistry into the Undergraduate Curriculum. Journal of Chemical Education, 2022, 99, 1428-1434.	1.1	4
2	Ligand-Induced Conformational and Dynamical Changes in a GT-B Glycosyltransferase: Molecular Dynamics Simulations of Heptosyltransferase I Complexes. Journal of Chemical Information and Modeling, 2022, 62, 324-339.	2.5	8
3	Discovery of first-in-class nanomolar inhibitors of heptosyltransferase I reveals a new aminoglycoside target and potential alternative mechanism of action. Scientific Reports, 2022, 12, 7302.	1.6	5
4	NAD+ enhances ribitol and ribose rescue of Î±-dystroglycan functional glycosylation in human FKRP-mutant myotubes. ELife, 2021, 10, .	2.8	9
5	CD200 Immune-Checkpoint Peptide Elicits an Anti-glioma Response Through the DAP10 Signaling Pathway. Neurotherapeutics, 2021, 18, 1980-1994.	2.1	6
6	Conserved Conformational Hierarchy across Functionally Divergent Glycosyltransferases of the GT-B Structural Superfamily as Determined from Microsecond Molecular Dynamics. International Journal of Molecular Sciences, 2021, 22, 4619.	1.8	10
7	Fragmentâ€based screening and hitâ€based substructure search: Rapid discovery of 8â€hydroxyquinolineâ€7â€carboxylic acid as a lowâ€cytotoxic, nanomolar metallo Î²â€lactamase inhibitor. Chemical Biology and Drug Design, 2021, 98, 481-492.	1.5	3
8	The molecular identity of the TLQP-21 peptide receptor. Cellular and Molecular Life Sciences, 2021, 78, 7133-7144.	2.4	3
9	CD200 Checkpoint Reversal: A Novel Approach to Immunotherapy. Clinical Cancer Research, 2020, 26, 232-241.	3.2	25
10	Opposites Attract: Escherichia coli Heptosyltransferase I Conformational Changes Induced by Interactions between the Substrate and Positively Charged Residues. Biochemistry, 2020, 59, 3135-3147.	1.2	11
11	Peptide/Receptor Co-evolution Explains the Lipolytic Function of the Neuropeptide TLQP-21. Cell Reports, 2019, 28, 2567-2580.e6.	2.9	20
12	Modeling and Simulation of hGAT1: A Mechanistic Investigation of the GABA Transport Process. Computational and Structural Biotechnology Journal, 2019, 17, 61-69.	1.9	4
13	TnI Structural Interface with the N-Terminal Lobe ofÂTnC as a Determinant of Cardiac Contractility. Biophysical Journal, 2018, 114, 1646-1656.	0.2	6
14	Can 5-methylcytosine analogues with extended alkyl side chains guide DNA methylation?. Chemical Communications, 2018, 54, 1061-1064.	2.2	10
15	Aptamer adaptive binding assessed by stilbene photoisomerization towards regenerating aptasensors. Sensors and Actuators B: Chemical, 2018, 257, 245-255.	4.0	21
16	Muscle membrane integrity in Duchenne muscular dystrophy: recent advances in copolymer-based muscle membrane stabilizers. Skeletal Muscle, 2018, 8, 31.	1.9	41
17	Maintenance DNA Methyltransferase Activity in the Presence of Oxidized Forms of 5-Methylcytosine: Structural Basis for Ten Eleven Translocation-Mediated DNA Demethylation. Biochemistry, 2018, 57, 6061-6069.	1.2	23
18	An Indoleâ€“Chalcone Inhibits Multidrug-Resistant Cancer Cell Growth by Targeting Microtubules. Molecular Pharmaceutics, 2018, 15, 3892-3900.	2.3	36

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19	The Stories Tryptophans Tell: Exploring Protein Dynamics of Heptosyltransferase I from Escherichia coli. Biochemistry, 2017, 56, 886-895.	1.2	20
20	Discovery of 1â€Hydroxypyridineâ€2(1H)â€thioneâ€6â€carboxylic Acid as a Firstâ€inâ€Class Lowâ€Cytotoxic Nanomolar Metallo Î²â€Lactamase Inhibitor. ChemMedChem, 2017, 12, 845-849.	1.6	18
21	Chemical End Group Modified Diblock Copolymers Elucidate Anchor and Chain Mechanism of Membrane Stabilization. Molecular Pharmaceutics, 2017, 14, 2333-2339.	2.3	28
22	All-Atom Molecular Dynamics-Based Analysis of Membrane-Stabilizing Copolymer Interactions with Lipid Bilayers Probed under Constant Surface Tensions. Journal of Physical Chemistry B, 2017, 121, 10657-10664.	1.2	27
23	Mosquito salivary allergen Aed a 3: cloning, comprehensive molecular analysis, and clinical evaluation. Allergy: European Journal of Allergy and Clinical Immunology, 2016, 71, 621-628.	2.7	18
24	Bypass of DNA-Protein Cross-links Conjugated to the 7-Deazaguanine Position of DNA by Translesion Synthesis Polymerases. Journal of Biological Chemistry, 2016, 291, 23589-23603.	1.6	33
25	Borrowing from the Platypus: Proline Substitution in Cardiac Troponin I. Biophysical Journal, 2015, 108, 447a.	0.2	0
26	Discovery of 1-hydroxypyridine-2-thiones as selective histone deacetylase inhibitors and their potential application for treating leukemia. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 4320-4324.	1.0	22
27	Inhibition of Inflammatory and Neuropathic Pain by Targeting a Mu Opioid Receptor/Chemokine Receptor5 Heteromer (MOR-CCR₅). Journal of Medicinal Chemistry, 2015, 58, 8647-8657.	2.9	53
28	Mutations in the Amino Terminus of Herpes Simplex Virus Type 1 gL Can Reduce Cell-Cell Fusion without Affecting gH/gL Trafficking. Journal of Virology, 2014, 88, 739-744.	1.5	4
29	Cell permeable vanX inhibitors as vancomycin re-sensitizing agents. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 2535-2538.	1.0	11
30	Rapid Identification of Keap1â€“Nrf2 Small-Molecule Inhibitors through Structure-Based Virtual Screening and Hit-Based Substructure Search. Journal of Medicinal Chemistry, 2014, 57, 1121-1126.	2.9	127
31	Molecular Determinants of Cardiac Myocyte Performance as Conferred by Isoform-Specific TnI Residues. Biophysical Journal, 2014, 106, 2105-2114.	0.2	11
32	A novel drug discovery strategy: Mechanistic investigation of an enantiomeric antitumor agent targeting dual p53 and NF-ÎºB pathways. Oncotarget, 2014, 5, 10830-10839.	0.8	11
33	Structure and Stability of Human Telomeric G-Quadruplex with Preclinical 9-Amino Acridines. PLoS ONE, 2013, 8, e57701.	1.1	21
34	5-Arylidenethioxothiazolidinones as Inhibitors of Tyrosylâ€“DNA Phosphodiesterase I. Journal of Medicinal Chemistry, 2012, 55, 8671-8684.	2.9	56
35	pH-Responsive Titratable Inotropic Performance of Histidine-Modified Cardiac Troponin I. Biophysical Journal, 2012, 102, 1570-1579.	0.2	12
36	Computational Studies of a pH Responsive Histidine-Modified Cardiac Troponin I. Biophysical Journal, 2012, 102, 736a.	0.2	0

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37	Molecular Mechanisms of A164H cTnI. Biophysical Journal, 2012, 102, 560a-561a.	0.2	0
38	The design, synthesis and biological evaluations of C-6 or C-7 substituted 2-hydroxyisoquinoline-1,3-diones as inhibitors of hepatitis C virus. Bioorganic and Medicinal Chemistry, 2012, 20, 467-479.	1.4	66
39	N-3 Hydroxylation of Pyrimidine-2,4-diones Yields Dual Inhibitors of HIV Reverse Transcriptase and Integrase. ACS Medicinal Chemistry Letters, 2011, 2, 63-67.	1.3	61
40	3-Hydroxypyrimidine-2,4-diones as an Inhibitor Scaffold of HIV Integrase. Journal of Medicinal Chemistry, 2011, 54, 2282-2292.	2.9	54
41	6-Benzoyl-3-hydroxypyrimidine-2,4-diones as dual inhibitors of HIV reverse transcriptase and integrase. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 2400-2402.	1.0	37
42	A continuous fluorescence displacement assay for BioA: An enzyme involved in biotin biosynthesis. Analytical Biochemistry, 2011, 416, 27-38.	1.1	17
43	pH-Dependent Transport of Pemetrexed by Breast Cancer Resistance Protein. Drug Metabolism and Disposition, 2011, 39, 1478-1485.	1.7	28
44	Design, asymmetric synthesis, and evaluation of pseudosymmetric sulfoximine inhibitors against HIV-1 protease. Bioorganic and Medicinal Chemistry, 2010, 18, 2037-2048.	1.4	35
45	Dual inhibitors of inosine monophosphate dehydrogenase and histone deacetylase based on a cinnamic hydroxamic acid core structure. Bioorganic and Medicinal Chemistry, 2010, 18, 5950-5964.	1.4	40
46	Scaffold rearrangement of dihydroxypyrimidine inhibitors of HIV integrase: Docking model revisited. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 3275-3279.	1.0	28
47	Pathogenic peptide deviations support a model of adaptive evolution of chordate cardiac performance by troponin mutations. Physiological Genomics, 2010, 42, 287-299.	1.0	20
48	Triazole-Linked Inhibitors of Inosine Monophosphate Dehydrogenase from Human and Mycobacterium tuberculosis. Journal of Medicinal Chemistry, 2010, 53, 4768-4778.	2.9	65
49	Selective inhibition of nicotinamide adenine dinucleotide kinases by dinucleoside disulfide mimics of nicotinamide adenine dinucleotide analogues. Bioorganic and Medicinal Chemistry, 2009, 17, 5656-5664.	1.4	21
50	Shared Catalysis in Virus Entry and Bacterial Cell Wall Depolymerization. Journal of Molecular Biology, 2009, 387, 607-618.	2.0	28
51	Design and synthesis of sulfoximine based inhibitors for HIV-1 protease. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 5406-5410.	1.0	31
52	CXC and CC Chemokines Form Mixed Heterodimers. Journal of Biological Chemistry, 2008, 283, 24155-24166.	1.6	65
53	Direct Inhibition of Insulin-Like Growth Factor-I Receptor Kinase Activity by (â^')â^'Epigallocatechin-3-Gallate Regulates Cell Transformation. Cancer Epidemiology Biomarkers and Prevention, 2007, 16, 598-605.	1.1	121
54	Impact of the C-Terminal Loop of Histidine Triad Nucleotide Binding Protein1 (Hint1) on Substrate Specificity. Biochemistry, 2007, 46, 13074-13079.	1.2	15

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55	A Universal Method for the Preparation of Covalent Proteinâ€“DNA Conjugates for Use in Creating Protein Nanostructures. Angewandte Chemie - International Edition, 2007, 46, 8819-8822.	7.2	103
56	Development of selective inhibitors for anti-apoptotic Bcl-2 proteins from BHI-1. Bioorganic and Medicinal Chemistry, 2007, 15, 2167-2176.	1.4	44
57	A critical role for the loop region of the basic helix-loop-helix/leucine zipper protein Mlx in DNA binding and glucose-regulated transcription. Nucleic Acids Research, 2006, 35, 35-44.	6.5	51
58	Amiodarone Analog-Dependent Effects on CYP2C9-Mediated Metabolism and Kinetic Profiles. Drug Metabolism and Disposition, 2006, 34, 1688-1696.	1.7	18
59	Homology Modeling and Molecular Dynamics Simulations of the Mu Opioid Receptor in a Membrane-Aqueous System. ChemBioChem, 2005, 6, 853-859.	1.3	46
60	Platelet Factor 4 and Interleukin-8 CXC Chemokine Heterodimer Formation Modulates Function at the Quaternary Structural Level. Journal of Biological Chemistry, 2005, 280, 4948-4958.	1.6	86
61	Blue Matter, an application framework for molecular simulation on Blue Gene. Journal of Parallel and Distributed Computing, 2003, 63, 759-773.	2.7	62
62	Thermal unfolding molecular dynamics simulation ofEscherichia coli dihydrofolate reductase: Thermal stability of protein domains and unfolding pathway. Proteins: Structure, Function and Bioinformatics, 2002, 46, 308-320.	1.5	39
63	Blue Gene: A vision for protein science using a petaflop supercomputer. IBM Systems Journal, 2001, 40, 310-327.	3.1	211
64	Protein Folding and Function: The N-Terminal Fragment in Adenylate Kinase. Biophysical Journal, 2001, 80, 2439-2454.	0.2	35
65	Structured disorder and conformational selection. Proteins: Structure, Function and Bioinformatics, 2001, 44, 418-427.	1.5	184
66	Molecular dynamics simulation of Escherichia coli dihydrofolate reductase and its protein fragments: Relative stabilities in experiment and simulations. Protein Science, 2001, 10, 135-148.	3.1	19
67	Examining methods for calculations of binding free energies: LRA, LIE, PDLD-LRA, and PDLD/S-LRA calculations of ligands binding to an HIV protease. Proteins: Structure, Function and Bioinformatics, 2000, 39, 393-407.	1.5	202
68	How important are entropic contributions to enzyme catalysis?. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 11899-11904.	3.3	178
69	Calculations of Activation Entropies of Chemical Reactions in Solution. Journal of Physical Chemistry B, 2000, 104, 4578-4584.	1.2	166
70	Examining methods for calculations of binding free energies: LRA, LIE, PDLD-LRA, and PDLD/S-LRA calculations of ligands binding to an HIV protease. , 2000, 39, 393.		4
71	Simulating proton translocations in proteins: Probing proton transfer pathways in theRhodobacter sphaeroides reaction center. Proteins: Structure, Function and Bioinformatics, 1999, 36, 484-500.	1.5	81
72	Simulating proton translocations in proteins: Probing proton transfer pathways in the Rhodobacter sphaeroides reaction center. , 1999, 36, 484.		1

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73	The Effect of Protein Relaxation on Charge-Charge Interactions and Dielectric Constants of Proteins. Biophysical Journal, 1998, 74, 1744-1753.	0.2	207
74	The surface constraint all atom model provides size independent results in calculations of hydration free energies. Journal of Chemical Physics, 1998, 109, 7940-7944.	1.2	60
75	Consistent Calculations of pKa's of Ionizable Residues in Proteins:â€‰ Semi-microscopic and Microscopic Approaches. Journal of Physical Chemistry B, 1997, 101, 4458-4472.	1.2	357
76	Temperature dependent near UV molar absorptivities of several small aldehydes in aqueous solution. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1995, 51, 247-251.	2.0	12
77	Case study: an environment for understanding protein simulations using game graphics. , 0, , .		1