Jerome Baudry

List of Publications by Year
in descending order

35 papers	1,316 citations	471061 17 h-index	377514 34 g-index
39 all docs	39 docs citations	39 times ranked	2058 citing authors

#	Article	IF	Citations
1	Ensemble Docking in Drug Discovery. Biophysical Journal, 2018, 114, 2271-2278.	0.2	318
2	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. Journal of Chemical Information and Modeling, 2020, 60, 5832-5852.	2.5	134
3	Evidence for Osteocalcin Binding and Activation of GPRC6A in Î²-Cells. Endocrinology, 2016, 157, 1866-1880.	1.4	101
4	Reviving Antibiotics: Efflux Pump Inhibitors That Interact with AcrA, a Membrane Fusion Protein of the AcrAB-TolC Multidrug Efflux Pump. ACS Infectious Diseases, 2017, 3, 89-98.	1.8	88
5	Ensemble Docking in Drug Discovery: How Many Protein Configurations from Molecular Dynamics Simulations are Needed To Reproduce Known Ligand Binding?. Journal of Physical Chemistry B, 2019, 123, 5189-5195.	1.2	69
6	VinaMPI: Facilitating multiple receptor high-throughput virtual docking on high-performance computers. Journal of Computational Chemistry, 2013, 34, 2212-2221.	1.5	62
7	Structural and Functional Evidence for Testosterone Activation of GPRC6A in Peripheral Tissues. Molecular Endocrinology, 2015, 29, 1759-1773.	3.7	52
8	Polycystin-1 interacts with TAZ to stimulate osteoblastogenesis and inhibit adipogenesis. Journal of Clinical Investigation, 2017, 128, 157-174.	3.9	49
9	Identification and Structureâ€“Activity Relationships of Novel Compounds that Potentiate the Activities of Antibiotics in Escherichia coli. Journal of Medicinal Chemistry, 2017, 60, 6205-6219.	2.9	45
10	Ensemble-based docking: From hit discovery to metabolism and toxicity predictions. Bioorganic and Medicinal Chemistry, 2016, 24, 4928-4935.	1.4	41
11	Structure-based design of broadly protective group a streptococcal M protein-based vaccines. Vaccine, 2017, 35, 19-26.	1.7	41
12	A phenylalanine rotameric switch for signal-state control in bacterial chemoreceptors. Nature Communications, 2013, 4, 2881.	5.8	37
13	A computationally identified compound antagonizes excess FGF-23 signaling in renal tubules and a mouse model of hypophosphatemia. Science Signaling, 2016, 9, ra113.	1.6	27
14	Ensemble docking to difficult targets in earlyâ€stage drug discovery: Methodology and application to fibroblast growth factor 23. Chemical Biology and Drug Design, 2018, 91, 491-504.	1.5	25
15	Novel Small Molecule JP-153 Targets the Src-FAK-Paxillin Signaling Complex to Inhibit VEGF-Induced Retinal Angiogenesis. Molecular Pharmacology, 2017, 91, 1-13.	1.0	23
16	Highâ€throughput virtual molecular docking with AutoDockCloud. Concurrency Computation Practice and Experience, 2014, 26, 907-916.	1.4	21
17	GPCR6A Is a Molecular Target for the Natural Products Gallate and EGCG in Green Tea. Molecular Nutrition and Food Research, 2018, 62, e1700770.	1.5	21
18	Computationally identified novel agonists for GPRC6A. PLoS ONE, 2018, 13, e0195980.	1.1	19

#	Article	IF	Citations
19	Discovery of Novel Nonactive Site Inhibitors of the Prothrombinase Enzyme Complex. Journal of Chemical Information and Modeling, 2016, 56, 535-547.	2.5	18
20	Polypharmacology and supercomputer-based docking: opportunities and challenges. Molecular Simulation, 2014, 40, 848-854.	0.9	16
21	Molecular interactions between photosystem I and ferredoxin: an integrated energy frustration and experimental model. Journal of Molecular Recognition, 2014, 27, 597-608.	1.1	13
22	Highly Dynamic Anionâ€“Quadrupole Networks in Proteins. Biochemistry, 2016, 55, 6056-6069.	1.2	11
23	Small Molecule Condensin Inhibitors. ACS Infectious Diseases, 2018, 4, 1737-1745.	1.8	10
24	The quinic acid derivative KZ-41 prevents glucose-induced caspase-3 activation in retinal endothelial cells through an IGF-1 receptor dependent mechanism. PLoS ONE, 2017, 12, e0180808.	1.1	10
25	General trends of dihedral conformational transitions in a globular protein. Proteins: Structure, Function and Bioinformatics, 2016, 84, 501-514.	1.5	8
26	Structure-based group A streptococcal vaccine design: Helical wheel homology predicts antibody cross-reactivity among streptococcal M proteinâ€“derived peptides. Journal of Biological Chemistry, 2020, 295, 3826-3836.	1.6	8
27	Discovery of an Inhibitor of Z-Alpha1 Antitrypsin Polymerization. PLoS ONE, 2015, 10, e0126256.	1.1	8
28	Accelerating virtual highâ€throughput ligand docking: current technology and case study on a petascale supercomputer. Concurrency Computation Practice and Experience, 2014, 26, 1268-1277.	1.4	7
29	Structure based virtual screening identifies small molecule effectors for the sialoglycan binding protein Hsa. Biochemical Journal, 2020, 477, 3695-3707.	1.7	7
30	The carboxylation status of osteocalcin has important consequences for its structure and dynamics. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129809.	1.1	5
31	Binding Mechanisms of Electron Transport Proteins with Cyanobacterial Photosystem I: An Integrated Computational and Experimental Model. Journal of Physical Chemistry B, 2018, 122, 1026-1036.	1.2	4
32	Ligand-Dependent Sodium Ion Dynamics within the A_{2A} Adenosine Receptor: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2019, 123, 7947-7954.	1.2	4
33	Cross-reactive immunogenicity of group A streptococcal vaccines designed using a recurrent neural network to identify conserved M protein linear epitopes. Vaccine, 2021, 39, 1773-1779.	1.7	4
34	Thermophilic Enzyme or Mesophilic Enzyme with Enhanced Thermostability: Can We Draw a Line?. Journal of Physical Chemistry B, 2017, 121, 7086-7094.	1.2	3
35	Editorial: Advances in computational molecular biophysics. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129888.	1.1	0