Jerome Baudry

List of Publications by Citations

35 papers	871 citations	15 h-index	29 g-index
39 ext. papers	1,114 ext. citations	4.6 avg, IF	4.25 L-index

#	Paper	IF	Citations
35	Ensemble Docking in Drug Discovery. *Biophysical Journal*, **2018**, 114, 2271-2278	2.9	203
34	Evidence for Osteocalcin Binding and Activation of GPRC6A in Cells. *Endocrinology*, **2016**, 157, 1866-80	4.8	78
33	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. *Journal of Chemical Information and Modeling*, **2020**, 60, 5832-5852	6.1	71
32	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	5.5	48
31	VinaMPI: facilitating multiple receptor high-throughput virtual docking on high-performance computers. *Journal of Computational Chemistry*, **2013**, 34, 2212-21	3.5	45
30	Structural and Functional Evidence for Testosterone Activation of GPRC6A in Peripheral Tissues. *Molecular Endocrinology*, **2015**, 29, 1759-73		43
29	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	3.4	42
28	Identification and Structure-Activity Relationships of Novel Compounds that Potentiate the Activities of Antibiotics in Escherichia coli. *Journal of Medicinal Chemistry*, **2017**, 60, 6205-6219	8.3	33
27	Polycystin-1 interacts with TAZ to stimulate osteoblastogenesis and inhibit adipogenesis. *Journal of Clinical Investigation*, **2018**, 128, 157-174	15.9	32
26	Structure-based design of broadly protective group a streptococcal M protein-based vaccines. *Vaccine*, **2017**, 35, 19-26	4.1	31
25	Ensemble-based docking: From hit discovery to metabolism and toxicity predictions. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4928-4935	3.4	30
24	A phenylalanine rotameric switch for signal-state control in bacterial chemoreceptors. *Nature Communications*, **2013**, 4, 2881	17.4	29
23	A computationally identified compound antagonizes excess FGF-23 signaling in renal tubules and a mouse model of hypophosphatemia. *Science Signaling*, **2016**, 9, ra113	8.8	19
22	High-throughput virtual molecular docking with AutoDockCloud. *Concurrency Computation Practice and Experience*, **2014**, 26, 907-916	1.4	18
21	Novel Small Molecule JP-153 Targets the Src-FAK-Paxillin Signaling Complex to Inhibit VEGF-Induced Retinal Angiogenesis. *Molecular Pharmacology*, **2017**, 91, 1-13	4.3	15
20	Ensemble docking to difficult targets in early-stage drug discovery: Methodology and application to fibroblast growth factor 23. *Chemical Biology and Drug Design*, **2018**, 91, 491-504	2.9	15
19	GPCR6A Is a Molecular Target for the Natural Products Gallate and EGCG in Green Tea. *Molecular Nutrition and Food Research*, **2018**, 62, e1700770	5.9	14

18	Discovery of Novel Nonactive Site Inhibitors of the Prothrombinase Enzyme Complex. *Journal of Chemical Information and Modeling*, **2016**, 56, 535-47	6.1	12
17	Computationally identified novel agonists for GPRC6A. *PLoS ONE*, **2018**, 13, e0195980	3.7	12
16	Molecular interactions between photosystem I and ferredoxin: an integrated energy frustration and experimental model. *Journal of Molecular Recognition*, **2014**, 27, 597-608	2.6	11
15	Polypharmacology and supercomputer-based docking: opportunities and challenges. *Molecular Simulation*, **2014**, 40, 848-854	2	10
14	Highly Dynamic Anion-Quadrupole Networks in Proteins. *Biochemistry*, **2016**, 55, 6056-6069	3.2	9
13	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	3.7	7
12	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. *ChemRxiv*, **2020**,	4.4	7
11	Discovery of an inhibitor of Z-alpha1 antitrypsin polymerization. *PLoS ONE*, **2015**, 10, e0126256	3.7	6
10	General trends of dihedral conformational transitions in a globular protein. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 501-14	4.2	6
9	Accelerating Virtual High-Throughput Ligand Docking: current technology and case study on a petascale supercomputer. *Concurrency Computation Practice and Experience*, **2014**, 26, 1268-1277	1.4	4
8	Structure based virtual screening identifies small molecule effectors for the sialoglycan binding protein Hsa. *Biochemical Journal*, **2020**, 477, 3695-3707	3.8	4
7	Small Molecule Condensin Inhibitors. *ACS Infectious Diseases*, **2018**, 4, 1737-1745	5.5	4
6	Structure-based group A streptococcal vaccine design: Helical wheel homology predicts antibody cross-reactivity among streptococcal M protein-derived peptides. *Journal of Biological Chemistry*, **2020**, 295, 3826-3836	5.4	3
5	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	3.4	3
4	Ligand-Dependent Sodium Ion Dynamics within the A Adenosine Receptor: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2019**, 123, 7947-7954	3.4	2
3	Thermophilic Enzyme or Mesophilic Enzyme with Enhanced Thermostability: Can We Draw a Line?. *Journal of Physical Chemistry B*, **2017**, 121, 7086-7094	3.4	2
2	The carboxylation status of osteocalcin has important consequences for its structure and dynamics. *Biochimica Et Biophysica Acta - General Subjects*, **2021**, 1865, 129809	4	2
1	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	4.1	1