Shuguang Yuan

List of Publications by Year in Descending Order

64 papers	2,491 citations	27 h-index	49 g-index
73 ext. papers	3,244 ext. citations	10.9 avg, IF	5.34 L-index

#	Paper	IF	Citations
64	Accurate Physical Property Predictions via Deep Learning.. *Molecules*, **2022**, 27,	4.8	1
63	Secondary-structure switch regulates the substrate binding of a YopJ family acetyltransferase. *Nature Communications*, **2021**, 12, 5969	17.4	1
62	Structure-Guided Rational Design of a Mono- and Diacylglycerol Lipase from : A Single Residue Mutant Increases the Hydrolysis Ability. *Journal of Agricultural and Food Chemistry*, **2021**, 69, 5344-5352	5.7	3
61	Asymmetric opening of the homopentameric 5-HT serotonin receptor in lipid bilayers. *Nature Communications*, **2021**, 12, 1074	17.4	8
60	Rutin, A Natural Inhibitor of IGPD Protein, Partially Inhibits Biofilm Formation in ATCC700404 and. *Frontiers in Pharmacology*, **2021**, 12, 728354	5.6	
59	Discovery of Traditional Chinese Medicines against Porcine Reproductive and Respiratory Syndrome Virus. *Pharmacological Research Modern Chinese Medicine*, **2021**, 100003		0
58	Enhancing the Signaling of GPCRs via Orthosteric Ions. *ACS Central Science*, **2020**, 6, 274-282	16.8	11
57	Activation and Signaling Mechanism Revealed by Cannabinoid Receptor-G Complex Structures. *Cell*, **2020**, 180, 655-665.e18	56.2	88
56	Discovering Anti-Cancer Drugs Computational Methods. *Frontiers in Pharmacology*, **2020**, 11, 733	5.6	52
55	Structure-guided engineering of a Thermobifida fusca cutinase for enhanced hydrolysis on natural polyester substrate. *Bioresources and Bioprocessing*, **2020**, 7,	5.2	4
54	Clinical HDAC Inhibitors Are Effective Drugs to Prevent the Entry of SARS-CoV2. *ACS Pharmacology and Translational Science*, **2020**, 3, 1361-1370	5.9	9
53	Structural basis of CXC chemokine receptor 2 activation and signalling. *Nature*, **2020**, 585, 135-140	50.4	50
52	Hatchet ribozyme structure and implications for cleavage mechanism. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 10783-10791	11.5	16
51	Computational modeling of the olfactory receptor Olfr73 suggests a molecular basis for low potency of olfactory receptor-activating compounds. *Communications Biology*, **2019**, 2, 141	6.7	12
50	Movements of the Substrate-Binding Clamp of Cypemycin Decarboxylase CypD. *Journal of Chemical Information and Modeling*, **2019**, 59, 2924-2929	6.1	5
49	Cover Image, Volume 9, Issue 4. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1431	7.9	
48	Advancing Drug Discovery via Artificial Intelligence. *Trends in Pharmacological Sciences*, **2019**, 40, 592-604	13.2	144

47	Modeling of Membrane Proteins. *Springer Series on Bio- and Neurosystems*, **2019**, 371-451	0.5	2
46	Molecular Mechanism for Ligand Recognition and Subtype Selectivity of Adrenergic Receptor. *Cell Reports*, **2019**, 29, 2936-2943.e4	10.6	5
45	New Binding Sites, New Opportunities for GPCR Drug Discovery. *Trends in Biochemical Sciences*, **2019**, 44, 312-330	10.3	72
44	Rationalization of stereoselectivity in enzyme reactions. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1403	7.9	2
43	5-HT Receptor Structures Reveal the Structural Basis of GPCR Polypharmacology. *Cell*, **2018**, 172, 719-736e14	36.2	123
42	Exploring a new ligand binding site of G protein-coupled receptors. *Chemical Science*, **2018**, 9, 6480-6489	9.4	33
41	Resistance-gene-directed discovery of a natural-product herbicide with a new mode of action. *Nature*, **2018**, 559, 415-418	50.4	108
40	Development of Photoaffinity Probe for the Discovery of Steviol Glycosides Biosynthesis Pathway in Stevia rebuadiana and Rapid Substrate Screening. *ACS Chemical Biology*, **2018**, 13, 1944-1949	4.9	22
39	Discovery of Arabidopsis UGT73C1 as a steviol-catalyzing UDP-glycosyltransferase with chemical probes. *Chemical Communications*, **2018**, 54, 7179-7182	5.8	8
38	Structural and Computational Insight into the Catalytic Mechanism of Limonene Epoxide Hydrolase Mutants in Stereoselective Transformations. *Journal of the American Chemical Society*, **2018**, 140, 310-318	16.4	30
37	Large conformational changes of a highly dynamic pre-protein binding domain in SecA. *Communications Biology*, **2018**, 1, 130	6.7	11
36	Cover Image, Volume 7, Issue 2. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1303	7.9	
35	Implementing WebGL and HTML5 in Macromolecular Visualization and Modern Computer-Aided Drug Design. *Trends in Biotechnology*, **2017**, 35, 559-571	15.1	21
34	Using PyMOL as a platform for computational drug design. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1298	7.9	98
33	Designing Safer Analgesics via Opioid Receptor Pathways. *Trends in Pharmacological Sciences*, **2017**, 38, 1016-1037	13.2	42
32	Investigating Substrate Scope and Enantioselectivity of a Defluorinase by a Stereochemical Probe. *Journal of the American Chemical Society*, **2017**, 139, 11241-11247	16.4	17
31	GyrI-like proteins catalyze cyclopropanoid hydrolysis to confer cellular protection. *Nature Communications*, **2017**, 8, 1485	17.4	6
30	Structure of a pathogen effector reveals the enzymatic mechanism of a novel acetyltransferase family. *Nature Structural and Molecular Biology*, **2016**, 23, 847-52	17.6	27

29	The Principles of Ligand Specificity on beta-2-adrenergic receptor. *Scientific Reports*, **2016**, 6, 34736	4.9	31
28	Mechanistic Studies on the Stereoselectivity of the Serotonin 5-HT1A Receptor. *Angewandte Chemie - International Edition*, **2016**, 55, 8661-5	16.4	23
27	Mechanistic Studies on the Stereoselectivity of the Serotonin 5-HT1A Receptor. *Angewandte Chemie*, **2016**, 128, 8803-8807	3.6	2
26	PyMOL and Inkscape Bridge the Data and the Data Visualization. *Structure*, **2016**, 24, 2041-2042	5.2	100
25	A Gating Mechanism of the Serotonin 5-HT3 Receptor. *Structure*, **2016**, 24, 816-825	5.2	35
24	The Molecular Mechanism of P2Y1 Receptor Activation. *Angewandte Chemie*, **2016**, 128, 10487-10491	3.6	0
23	The Molecular Mechanism of P2Y1 Receptor Activation. *Angewandte Chemie - International Edition*, **2016**, 55, 10331-5	16.4	41
22	Mechanistic study of the radical SAM-dependent amine dehydrogenation reactions. *Chemical Communications*, **2016**, 52, 10555-8	5.8	23
21	W2466.48 Opens a Gate for a Continuous Intrinsic Water Pathway during Activation of the Adenosine A2A Receptor. *Angewandte Chemie*, **2015**, 127, 566-569	3.6	13
20	Exchanging ligand-binding specificity between a pair of mouse olfactory receptor paralogs reveals odorant recognition principles. *Scientific Reports*, **2015**, 5, 14948	4.9	17
19	The mechanism of ligand-induced activation or inhibition of □and □pioid receptors. *Angewandte Chemie - International Edition*, **2015**, 54, 7560-3	16.4	39
18	The Mechanism of Ligand-Induced Activation or Inhibition of □and □Opioid Receptors. *Angewandte Chemie*, **2015**, 127, 7670-7673	3.6	5
17	W246(6.48) opens a gate for a continuous intrinsic water pathway during activation of the adenosine A2A receptor. *Angewandte Chemie - International Edition*, **2015**, 54, 556-9	16.4	46
16	Engineering of an epoxide hydrolase for efficient bioresolution of bulky pharmaco substrates. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 15717-22	11.5	54
15	Advances in GPCR modeling evaluated by the GPCR Dock 2013 assessment: meeting new challenges. *Structure*, **2014**, 22, 1120-1139	5.2	136
14	Activation of G-protein-coupled receptors correlates with the formation of a continuous internal water pathway. *Nature Communications*, **2014**, 5, 4733	17.4	157
13	Modeling of Membrane Proteins. *Springer Series in Bio-/neuroinformatics*, **2014**, 357-431		
12	The role of water and sodium ions in the activation of the □pioid receptor. *Angewandte Chemie - International Edition*, **2013**, 52, 10112-5	16.4	86

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11	Enhancing the production of galacto-oligosaccharides by mutagenesis of Sulfolobus solfataricus β-galactosidase. *Food Chemistry*, **2013**, 138, 1588-95	8.5	52
10	Lipid receptor S1P1 activation scheme concluded from microsecond all-atom molecular dynamics simulations. *PLoS Computational Biology*, **2013**, 9, e1003261	5	25
9	Understanding the role of defective invertases in plants: tobacco Nin88 fails to degrade sucrose. *Plant Physiology*, **2013**, 161, 1670-81	6.6	45
8	Rolle des Wassers und der Natriumionen bei der Aktivierung des μ-Opioidrezeptors. *Angewandte Chemie*, **2013**, 125, 10299-10302	3.6	12
7	Crystal structure of 6-SST/6-SFT from Pachysandra terminalis, a plant fructan biosynthesizing enzyme in complex with its acceptor substrate 6-kestose. *Plant Journal*, **2012**, 70, 205-19	6.9	39
6	pKa modulation of the acid/base catalyst within GH32 and GH68: a role in substrate/inhibitor specificity?. *PLoS ONE*, **2012**, 7, e37453	3.7	16
5	The role of water in activation mechanism of human N-formyl peptide receptor 1 (FPR1) based on molecular dynamics simulations. *PLoS ONE*, **2012**, 7, e47114	3.7	21
4	Action of molecular switches in GPCRs--theoretical and experimental studies. *Current Medicinal Chemistry*, **2012**, 19, 1090-109	4.3	298
3	Molecular basis of LMAN1 in coordinating LMAN1-MCFD2 cargo receptor formation and ER-to-Golgi transport of FV/FVIII. *Blood*, **2010**, 116, 5698-706	2.2	47
2	Donor deficiency of decay-accelerating factor accelerates murine T cell-mediated cardiac allograft rejection. *Journal of Immunology*, **2008**, 181, 4580-9	5.3	81
1	The role of metal ions in G protein-coupled receptor signalling and drug discovery. *Wiley Interdisciplinary Reviews: Computational Molecular Science*,e1565	7.9	0