Shaoyong Lu

List of Publications by Year
in descending order

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94 papers	4,590 citations	87888 38 h-index	118850 62 g-index
94 all docs	94 docs citations	94 times ranked	3707 citing authors

#	Article	IF	Citations
1	Targeting a cryptic allosteric site of SIRT6 with small-molecule inhibitors that inhibit the migration of pancreatic cancer cells. Acta Pharmaceutica Sinica B, 2022, 12, 876-889.	12.0	32
2	Along the allostery stream: Recent advances in computational methods for allosteric drug discovery. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1585.	14.6	23
3	Delineating the activation mechanism and conformational landscape of a class B G protein-coupled receptor glucagon receptor. Computational and Structural Biotechnology Journal, 2022, 20, 628-639.	4.1	40
4	Explaining and Predicting Allostery with Allosteric Database and Modern Analytical Techniques. Journal of Molecular Biology, 2022, 434, 167481.	4.2	10
5	Elucidation of the conformational dynamics and assembly of Argonauteâ€“RNA complexes by distinct yet coordinated actions of the supplementary microRNA. Computational and Structural Biotechnology Journal, 2022, 20, 1352-1365.	4.1	13
6	Mechanistic Insights Into Co-Administration of Allosteric and Orthosteric Drugs to Overcome Drug-Resistance in T315I BCR-ABL1. Frontiers in Pharmacology, 2022, 13, 862504.	3.5	11
7	Computational elucidation of allosteric communication in proteins for allosteric drug design. Drug Discovery Today, 2022, 27, 2226-2234.	6.4	14
8	Beyond a Linker: The Role of Photochemistry of Crosslinkers in the Direct Optical Patterning of Colloidal Nanocrystals. Angewandte Chemie, 2022, 134, .	2.0	1
9	Autopromotion of K-Ras4B Feedback Activation Through an SOS-Mediated Long-Range Allosteric Effect. Frontiers in Molecular Biosciences, 2022, 9, 860962.	3.5	10
10	Hidden allosteric sites and De-Novo drug design. Expert Opinion on Drug Discovery, 2022, 17, 283-295.	5.0	13
11	Delineating the conformational landscape and intrinsic properties of the angiotensin II type 2 receptor using a computational study. Computational and Structural Biotechnology Journal, 2022, 20, 2268-2279.	4.1	4
12	Insights into the Allosteric Effect of SENP1 Q597A Mutation on the Hydrolytic Reaction of SUMO1 via an Integrated Computational Study. Molecules, 2022, 27, 4149.	3.8	4
13	Cover Image, Volume 12, Issue 4. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	0
14	Discovery of cryptic allosteric sites using reversed allosteric communication by a combined computational and experimental strategy. Chemical Science, 2021, 12, 464-476.	7.4	84
15	Allosteric binding sites at the receptorâ€“lipid bilayer interface: novel targets for GPCR drug discovery. Drug Discovery Today, 2021, 26, 690-703.	6.4	34
16	Mechanism of allosteric activation of SIRT6 revealed by the action of rationally designed activators. Acta Pharmaceutica Sinica B, 2021, 11, 1355-1361.	12.0	57
17	Dual roles of ATP-binding site in protein kinases: Orthosteric inhibition and allosteric regulation. Advances in Protein Chemistry and Structural Biology, 2021, 124, 87-119.	2.3	10
18	Mechanism of zinc ejection by disulfiram in nonstructural protein 5A. Physical Chemistry Chemical Physics, 2021, 23, 12204-12215.	2.8	22

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19	Mechanistic insights into the effect of phosphorylation on Ras conformational dynamics and its interactions with cell signaling proteins. Computational and Structural Biotechnology Journal, 2021, 19, 1184-1199.	4.1	51
20	Targeting RAS phosphorylation in cancer therapy: Mechanisms and modulators. Acta Pharmaceutica Sinica B, 2021, 11, 3433-3446.	12.0	20
21	Conformational Selection Mechanism Provides Structural Insights into the Optimization of APC-Asef Inhibitors. Molecules, 2021, 26, 962.	3.8	11
22	Advances and Insights of APC-Asef Inhibitors for Metastatic Colorectal Cancer Therapy. Frontiers in Molecular Biosciences, 2021, 8, 662579.	3.5	7
23	Untangling Dual-Targeting Therapeutic Mechanism of Epidermal Growth Factor Receptor (EGFR) Based on Reversed Allosteric Communication. Pharmaceutics, 2021, 13, 747.	4.5	42
24	Rational Design of Peptide-Based Inhibitors Disrupting Protein-Protein Interactions. Frontiers in Chemistry, 2021, 9, 682675.	3.6	54
25	Structure of an inactive conformation of GTP-bound RhoA GTPase. Structure, 2021, 29, 553-563.e5.	3.3	14
26	Tribute to Ruth Nussinov. Journal of Physical Chemistry B, 2021, 125, 6733-6734.	2.6	0
27	Activation pathway of a G protein-coupled receptor uncovers conformational intermediates as targets for allosteric drug design. Nature Communications, 2021, 12, 4721.	12.8	124
28	Identification of an allosteric hotspot for additive activation of PPARÎ³ in antidiabetic effects. Science Bulletin, 2021, 66, 1559-1570.	9.0	18
29	Markov State Models and Molecular Dynamics Simulations Provide Understanding of the Nucleotide-Dependent Dimerization-Based Activation of LRRK2 ROC Domain. Molecules, 2021, 26, 5647.	3.8	10
30	Transcriptome aberration in mice uterus associated with steroid hormone response and inflammation induced by dioxybenzone and its metabolites. Environmental Pollution, 2021, 286, 117294.	7.5	3
31	Predicting Multi-Interfacial Binding Mechanisms of NLRP3 and ASC Pyrin Domains in Inflammasome Activation. ACS Chemical Neuroscience, 2021, 12, 603-612.	3.5	10
32	Atomic-scale insights into allosteric inhibition and evolutional rescue mechanism of Streptococcus thermophilus Cas9 by the anti-CRISPR protein AcrIIA6. Computational and Structural Biotechnology Journal, 2021, 19, 6108-6124.	4.1	35
33	Harnessing Reversed Allosteric Communication: A Novel Strategy for Allosteric Drug Discovery. Journal of Medicinal Chemistry, 2021, 64, 17728-17743.	6.4	29
34	Deciphering the Mechanism of Gilteritinib Overcoming Lorlatinib Resistance to the Double Mutant I1171N/F1174I in Anaplastic Lymphoma Kinase. Frontiers in Cell and Developmental Biology, 2021, 9, 808864.	3.7	14
35	Unraveling allosteric landscapes of allosterome with ASD. Nucleic Acids Research, 2020, 48, D394-D401.	14.5	29
36	How does the novel T315L mutation of breakpoint cluster region-abelson (BCR-ABL) kinase confer resistance to ponatinib: a comparative molecular dynamics simulation study. Journal of Biomolecular Structure and Dynamics, 2020, 38, 89-100.	3.5	9

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37	Emergence of allosteric drug-resistance mutations: new challenges for allosteric drug discovery. Drug Discovery Today, 2020, 25, 177-184.	6.4	67
38	Insight into the mechanism of allosteric activation of PI3KÎ± by oncoprotein K-Ras4B. International Journal of Biological Macromolecules, 2020, 144, 643-655.	7.5	36
39	Computational methods-guided design of modulators targeting protein-protein interactions (PPIs). European Journal of Medicinal Chemistry, 2020, 207, 112764.	5.5	26
40	Zinc-mediated conformational preselection mechanism in the allosteric control of DNA binding to the zinc transcriptional regulator (ZitR). Scientific Reports, 2020, 10, 13276.	3.3	6
41	Pentabromoethylbenzene Exposure Induces Transcriptome Aberration and Thyroid Dysfunction: In Vitro, in Silico, and in Vivo Investigations. Environmental Science & Technology, 2020, 54, 12335-12344.	10.0	45
42	How Parkinson's disease-related mutations disrupt the dimerization of WD40 domain in LRRK2: a comparative molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2020, 22, 20421-20433.	2.8	13
43	Combining Allosteric and Orthosteric Drugs to Overcome Drug Resistance. Trends in Pharmacological Sciences, 2020, 41, 336-348.	8.7	60
44	Decoding allosteric communication pathways in protein lysine acetyltransferase. International Journal of Biological Macromolecules, 2020, 149, 70-80.	7.5	26
45	Molecular dynamics simulations provide insights into the origin of gleevecâ€™s selectivity toward human tyrosine kinases. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2733-2744.	3.5	17
46	Deactivation Pathway of Ras GTPase Underlies Conformational Substates as Targets for Drug Design. ACS Catalysis, 2019, 9, 7188-7196.	11.2	77
47	Allosteric Methods and Their Applications: Facilitating the Discovery of Allosteric Drugs and the Investigation of Allosteric Mechanisms. Accounts of Chemical Research, 2019, 52, 492-500.	15.6	132
48	The chemical diversity and structure-based discovery of allosteric modulators for the PIF-pocket of protein kinase PDK1. Journal of Enzyme Inhibition and Medicinal Chemistry, 2019, 34, 361-374.	5.2	19
49	Drugging K-RasG12C through covalent inhibitors: Mission possible?. , 2019, 202, 1-17.		63
50	AlloDriver: a method for the identification and analysis of cancer driver targets. Nucleic Acids Research, 2019, 47, W315-W321.	14.5	31
51	Metabolic intermediate acetyl phosphate modulates bacterial virulence via acetylation. Emerging Microbes and Infections, 2019, 8, 55-69.	6.5	37
52	Emerging roles of allosteric modulators in the regulation of proteinâ€protein interactions (PPIs): A new paradigm for PPI drug discovery. Medicinal Research Reviews, 2019, 39, 2314-2342.	10.5	77
53	Allosteric Modulator Discovery: From Serendipity to Structure-Based Design. Journal of Medicinal Chemistry, 2019, 62, 6405-6421.	6.4	124
54	Identification of a natural inhibitor of methionine adenosyltransferase 2A regulating one-carbon metabolism in keratinocytes. EBioMedicine, 2019, 39, 575-590.	6.1	19

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55	Are the Apo Proteins Suitable for the Rational Discovery of Allosteric Drugs?. Journal of Chemical Information and Modeling, 2019, 59, 597-604.	5.4	18
56	Small Molecule Allosteric Modulators of G-Protein-Coupled Receptors: Drugâ€“Target Interactions. Journal of Medicinal Chemistry, 2019, 62, 24-45.	6.4	114
57	Characteristics of Allosteric Proteins, Sites, and Modulators. Advances in Experimental Medicine and Biology, 2019, 1163, 107-139.	1.6	17
58	Progress in Allosteric Database. Advances in Experimental Medicine and Biology, 2019, 1163, 65-87.	1.6	5
59	Discovery of hidden allosteric sites as novel targets for allosteric drug design. Drug Discovery Today, 2018, 23, 359-365.	6.4	92
60	Identification of a cellularly active SIRT6 allosteric activator. Nature Chemical Biology, 2018, 14, 1118-1126.	8.0	193
61	Computational Insights into the Interactions between Calmodulin and the c/nSH2 Domains of p85Î± Regulatory Subunit of PI3KÎ±: Implication for PI3KÎ± Activation by Calmodulin. International Journal of Molecular Sciences, 2018, 19, 151.	4.1	23
62	AlloFinder: a strategy for allosteric modulator discovery and allosterome analyses. Nucleic Acids Research, 2018, 46, W451-W458.	14.5	79
63	Calmodulin and PI3K Signaling in KRAS Cancers. Trends in Cancer, 2017, 3, 214-224.	7.4	58
64	Germline Mutations in CDH23, Encoding Cadherin-Related 23, Are Associated with Both Familial and Sporadic Pituitary Adenomas. American Journal of Human Genetics, 2017, 100, 817-823.	6.2	57
65	Microsecond molecular dynamics simulations provide insight into the ATPâ€competitive inhibitorâ€induced allosteric protection of Akt kinase phosphorylation. Chemical Biology and Drug Design, 2017, 89, 723-731.	3.2	12
66	Improved Method for the Identification and Validation of Allosteric Sites. Journal of Chemical Information and Modeling, 2017, 57, 2358-2363.	5.4	93
67	Peptidomimetic inhibitors of APCâ€“Asef interaction block colorectal cancer migration. Nature Chemical Biology, 2017, 13, 994-1001.	8.0	79
68	Designed covalent allosteric modulators: an emerging paradigm in drug discovery. Drug Discovery Today, 2017, 22, 447-453.	6.4	44
69	Molecular Dynamics Simulations and Dynamic Network Analysis Reveal the Allosteric Unbinding of Monobody to H-Ras Triggered by R135K Mutation. International Journal of Molecular Sciences, 2017, 18, 2249.	4.1	23
70	Drugging Ras GTPase: a comprehensive mechanistic and signaling structural view. Chemical Society Reviews, 2016, 45, 4929-4952.	38.1	150
71	Inhibitors of Rasâ€“SOS Interactions. ChemMedChem, 2016, 11, 814-821.	3.2	62
72	Allosteric modulators of MEK1: drug design and discovery. Chemical Biology and Drug Design, 2016, 88, 485-497.	3.2	18

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73	The Structural Basis of Oncogenic Mutations G12, G13 and Q61 in Small GTPase K-Ras4B. Scientific Reports, 2016, 6, 21949.	3.3	149
74	The higher level of complexity of Kâ€Ras4B activation at the membrane. FASEB Journal, 2016, 30, 1643-1655.	0.5	73
75	BitterX: a tool for understanding bitter taste in humans. Scientific Reports, 2016, 6, 23450.	3.3	53
76	Ras Conformational Ensembles, Allostery, and Signaling. Chemical Reviews, 2016, 116, 6607-6665.	47.7	290
77	Alloscore: a method for predicting allosteric ligandâ€“protein interactions. Bioinformatics, 2016, 32, 1574-1576.	4.1	31
78	ASD v3.0: unraveling allosteric regulation with structural mechanisms and biological networks. Nucleic Acids Research, 2016, 44, D527-D535.	14.5	116
79	GTP Binding and Oncogenic Mutations May Attenuate Hypervariable Region (HVR)-Catalytic Domain Interactions in Small GTPase K-Ras4B, Exposing the Effector Binding Site. Journal of Biological Chemistry, 2015, 290, 28887-28900.	3.4	73
80	ASBench: benchmarking sets for allosteric discovery. Bioinformatics, 2015, 31, 2598-2600.	4.1	88
81	Prediction of Human Clearance Based on Animal Data and Molecular Properties. Chemical Biology and Drug Design, 2015, 86, 990-997.	3.2	13
82	The Mechanism of ATP-Dependent Allosteric Protection of Akt Kinase Phosphorylation. Structure, 2015, 23, 1725-1734.	3.3	58
83	The Mechanism of Allosteric Inhibition of Protein Tyrosine Phosphatase 1B. PLoS ONE, 2014, 9, e97668.	2.5	49
84	The Structural Basis of ATP as an Allosteric Modulator. PLoS Computational Biology, 2014, 10, e1003831.	3.2	76
85	Harnessing Allostery: A Novel Approach to Drug Discovery. Medicinal Research Reviews, 2014, 34, 1242-1285.	10.5	120
86	ASD v2.0: updated content and novel features focusing on allosteric regulation. Nucleic Acids Research, 2014, 42, D510-D516.	14.5	96
87	Crystal Structures of PI3KÎ± Complexed with PI103 and Its Derivatives: New Directions for Inhibitors Design. ACS Medicinal Chemistry Letters, 2014, 5, 138-142.	2.8	81
88	Recent computational advances in the identification of allosteric sites in proteins. Drug Discovery Today, 2014, 19, 1595-1600.	6.4	93
89	Structural basis of valmerins as dual inhibitors of GSK3Î²/CDK5. Journal of Molecular Modeling, 2014, 20, 2407.	1.8	27
90	Allosite: a method for predicting allosteric sites. Bioinformatics, 2013, 29, 2357-2359.	4.1	153

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91	Toward an understanding of the sequence and structural basis of allosteric proteins. Journal of Molecular Graphics and Modelling, 2013, 40, 30-39.	2.4	27
92	Insights into the Role of Magnesium Triad in myo-Inositol Monophosphatase: Metal Mechanism, Substrate Binding, and Lithium Therapy. Journal of Chemical Information and Modeling, 2012, 52, 2398-2409.	5.4	24
93	Mechanism of kinase inactivation and nonbinding of fratide to GSK3Î² due to K85M mutation: Molecular dynamics simulation and normal mode analysis. Biopolymers, 2011, 95, 669-681.	2.4	19
94	The Role of Conformational Dynamics and Allostery in the Control of Distinct Efficacies of Agonists to the Glucocorticoid Receptor. Frontiers in Molecular Biosciences, 0, 9, .	3.5	7