Yinglong Miao

List of Publications by Citations

85 papers	3,018 citations	31 h-index	54 g-index
117 ext. papers	3,984 ext. citations	5.3 avg, IF	6.02 L-index

#	Paper	IF	Citations
85	Gaussian Accelerated Molecular Dynamics: Unconstrained Enhanced Sampling and Free Energy Calculation. *Journal of Chemical Theory and Computation*, **2015**, 11, 3584-3595	6.4	302
84	Improved Reweighting of Accelerated Molecular Dynamics Simulations for Free Energy Calculation. *Journal of Chemical Theory and Computation*, **2014**, 10, 2677-2689	6.4	225
83	Ensemble Docking in Drug Discovery. *Biophysical Journal*, **2018**, 114, 2271-2278	2.9	203
82	Activation and dynamic network of the M2 muscarinic receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 10982-7	11.5	174
81	Accelerated molecular dynamics simulations of protein folding. *Journal of Computational Chemistry*, **2015**, 36, 1536-49	3.5	106
80	Accelerated molecular dynamics simulations of ligand binding to a muscarinic G-protein-coupled receptor. *Quarterly Reviews of Biophysics*, **2015**, 48, 479-87	7	100
79	Unconstrained Enhanced Sampling for Free Energy Calculations of Biomolecules: A Review. *Molecular Simulation*, **2016**, 42, 1046-1055	2	93
78	CRISPR-Cas9 conformational activation as elucidated from enhanced molecular simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 7260-7265	11.5	91
77	Graded activation and free energy landscapes of a muscarinic G-protein-coupled receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 12162-12167	11.5	79
76	Population based reweighting of scaled molecular dynamics. *Journal of Physical Chemistry B*, **2013**, 117, 12759-68	3.4	75
75	Accelerated structure-based design of chemically diverse allosteric modulators of a muscarinic G protein-coupled receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E5675-84	11.5	69
74	Striking Plasticity of CRISPR-Cas9 and Key Role of Non-target DNA, as Revealed by Molecular Simulations. *ACS Central Science*, **2016**, 2, 756-763	16.8	67
73	Gaussian Accelerated Molecular Dynamics in NAMD. *Journal of Chemical Theory and Computation*, **2017**, 13, 9-19	6.4	64
72	Mechanism of the G-protein mimetic nanobody binding to a muscarinic G-protein-coupled receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 3036-3041	11.5	64
71	Free energy landscape of G-protein coupled receptors, explored by accelerated molecular dynamics. *Physical Chemistry Chemical Physics*, **2014**, 16, 6398-406	3.6	62
70	G-protein coupled receptors: advances in simulation and drug discovery. *Current Opinion in Structural Biology*, **2016**, 41, 83-89	8.1	60
69	Deciphering Off-Target Effects in CRISPR-Cas9 through Accelerated Molecular Dynamics. *ACS Central Science*, **2019**, 5, 651-662	16.8	57

68	Allosteric effects of sodium ion binding on activation of the m3 muscarinic g-protein-coupled receptor. *Biophysical Journal*, **2015**, 108, 1796-1806	2.9	53
67	Mechanistic Insights into Specific G Protein Interactions with Adenosine Receptors. *Journal of Physical Chemistry B*, **2019**, 123, 6462-6473	3.4	51
66	All-atom multiscale simulation of cowpea chlorotic mottle virus capsid swelling. *Journal of Physical Chemistry B*, **2010**, 114, 11181-95	3.4	51
65	Gaussian Accelerated Molecular Dynamics: Theory, Implementation, and Applications. *Annual Reports in Computational Chemistry*, **2017**, 13, 231-278	1.8	47
64	Multi-conformer ensemble docking to difficult protein targets. *Journal of Physical Chemistry B*, **2015**, 119, 1026-34	3.4	46
63	Derivation of mean-square displacements for protein dynamics from elastic incoherent neutron scattering. *Journal of Physical Chemistry B*, **2012**, 116, 5028-36	3.4	40
62	Temperature-dependent dynamical transitions of different classes of amino acid residue in a globular protein. *Journal of the American Chemical Society*, **2012**, 134, 19576-9	16.4	38
61	Structural Basis for Binding of Allosteric Drug Leads in the Adenosine A Receptor. *Scientific Reports*, **2018**, 8, 16836	4.9	38
60	Mapping of allosteric druggable sites in activation-associated conformers of the M2 muscarinic receptor. *Chemical Biology and Drug Design*, **2014**, 83, 237-46	2.9	36
59	Peptide Gaussian accelerated molecular dynamics (Pep-GaMD): Enhanced sampling and free energy and kinetics calculations of peptide binding. *Journal of Chemical Physics*, **2020**, 153, 154109	3.9	36
58	Viral structural transitions: an all-atom multiscale theory. *Journal of Chemical Physics*, **2006**, 125, 214901	3.9	34
57	Ligand Binding Pathways and Conformational Transitions of the HIV Protease. *Biochemistry*, **2018**, 57, 1533-1541	3.2	33
56	Stochastic dynamics of bionanosystems: Multiscale analysis and specialized ensembles. *Journal of Chemical Physics*, **2008**, 128, 234908	3.9	32
55	Identification of SLAC1 anion channel residues required for CO/bicarbonate sensing and regulation of stomatal movements. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 11129-11137	11.5	32
54	All-atom multiscaling and new ensembles for dynamical nanoparticles. *Journal of Chemical Physics*, **2006**, 125, 44901	3.9	31
53	Ligand Gaussian Accelerated Molecular Dynamics (LiGaMD): Characterization of Ligand Binding Thermodynamics and Kinetics. *Journal of Chemical Theory and Computation*, **2020**, 16, 5526-5547	6.4	31
52	Improved Modeling of Peptide-Protein Binding Through Global Docking and Accelerated Molecular Dynamics Simulations. *Frontiers in Molecular Biosciences*, **2019**, 6, 112	5.6	29
51	Molecular dynamics/order parameter extrapolation for bionanosystem simulations. *Journal of Computational Chemistry*, **2009**, 30, 423-37	3.5	29

50	Gaussian accelerated molecular dynamics (GaMD): principles and applications.. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1521	7.9	28
49	Self-assembly of nanocomponents into composite structures: derivation and simulation of Langevin equations. *Journal of Chemical Physics*, **2009**, 130, 194115	3.9	24
48	Acceleration of biomolecular kinetics in Gaussian accelerated molecular dynamics. *Journal of Chemical Physics*, **2018**, 149, 072308	3.9	24
47	Coupled flexibility change in cytochrome P450cam substrate binding determined by neutron scattering, NMR, and molecular dynamics simulation. *Biophysical Journal*, **2012**, 103, 2167-76	2.9	22
46	Active-site hydration and water diffusion in cytochrome P450cam: a highly dynamic process. *Biophysical Journal*, **2011**, 101, 1493-503	2.9	22
45	Replica Exchange Gaussian Accelerated Molecular Dynamics: Improved Enhanced Sampling and Free Energy Calculation. *Journal of Chemical Theory and Computation*, **2018**, 14, 1853-1864	6.4	21
44	G-Protein-Coupled Receptor-Membrane Interactions Depend on the Receptor Activation State. *Journal of Computational Chemistry*, **2020**, 41, 460-471	3.5	21
43	Gaussian accelerated molecular dynamics for elucidation of drug pathways. *Expert Opinion on Drug Discovery*, **2018**, 13, 1055-1065	6.2	21
42	Mapping the allosteric sites of the A adenosine receptor. *Chemical Biology and Drug Design*, **2018**, 91, 5-16	2.9	18
41	Viral structural transition mechanisms revealed by multiscale molecular dynamics/order parameter extrapolation simulation. *Biopolymers*, **2010**, 93, 61-73	2.2	17
40	Reactive Center Loop Insertion in 1-Antitrypsin Captured by Accelerated Molecular Dynamics Simulation. *Biochemistry*, **2017**, 56, 634-646	3.2	16
39	Space warping order parameters and symmetry: application to multiscale simulation of macromolecular assemblies. *Journal of Physical Chemistry B*, **2012**, 116, 8423-34	3.4	16
38	Molecular dynamic study of MlaC protein in Gram-negative bacteria: conformational flexibility, solvent effect and protein-phospholipid binding. *Protein Science*, **2016**, 25, 1430-7	6.3	15
37	Quasielastic neutron scattering in biology: Theory and applications. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 3638-3650	4	12
36	Pathway and mechanism of drug binding to chemokine receptors revealed by accelerated molecular simulations. *Future Medicinal Chemistry*, **2020**, 12, 1213-1225	4.1	12
35	Mechanisms of Secretase Activation and Substrate Processing. *ACS Central Science*, **2020**, 6, 969-983	16.8	12
34	A Computational Modeling Approach Predicts Interaction of the Antifungal Protein AFP from with Fungal Membranes via Its Core Motif. *MSphere*, **2018**, 3,	5	12
33	Positive allosteric mechanisms of adenosine A receptor-mediated analgesia. *Nature*, **2021**, 597, 571-576	50.4	12

32	Activation mechanisms of the first sphingosine-1-phosphate receptor. *Protein Science*, **2017**, 26, 1150-1160	6.9	11
31	Structure of the Human Respiratory Syncytial Virus M2-1 Protein in Complex with a Short Positive-Sense Gene-End RNA. *Structure*, **2020**, 28, 979-990.e4	5.2	11
30	Investigation of the conformational dynamics of the apo A2A adenosine receptor. *Protein Science*, **2015**, 24, 1004-12	6.3	10
29	Ligand Binding in the Extracellular Vestibule of the Neurotransmitter Transporter Homologue LeuT. *ACS Chemical Neuroscience*, **2017**, 8, 619-628	5.7	9
28	Retrospective ensemble docking of allosteric modulators in an adenosine G-protein-coupled receptor. *Biochimica Et Biophysica Acta - General Subjects*, **2020**, 1864, 129615	4	8
27	Mechanism of RNA recognition by a Musashi RNA-binding protein.. *Current Research in Structural Biology*, **2022**, 4, 10-20	2.8	6
26	General trends of dihedral conformational transitions in a globular protein. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 501-14	4.2	6
25	Recent advances in computational studies of GPCR-G protein interactions. *Advances in Protein Chemistry and Structural Biology*, **2019**, 116, 397-419	5.3	5
24	Zaccai neutron resilience and site-specific hydration dynamics in a globular protein. *European Physical Journal E*, **2013**, 36, 72	1.5	5
23	Agonist Binding and G Protein Coupling in Histamine H Receptor: A Molecular Dynamics Study. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	5
22	Molecular mechanism of off-target effects in CRISPR-Cas9		4
21	Computer-aided GPCR drug discovery **2020**, 283-293		3
20	Identification and Validation of an Secondary Metabolite Derivative as an Inhibitor of the Musashi-RNA Interaction. *Cancers*, **2020**, 12,	6.6	3
19	Mechanism of Ligand Recognition by Human ACE2 Receptor. *Journal of Physical Chemistry Letters*, **2021**, 12, 4814-4822	6.4	3
18	Binding Analysis Using Accelerated Molecular Dynamics Simulations and Future Perspectives.. *Advances and Applications in Bioinformatics and Chemistry*, **2022**, 15, 1-19	1.5	2
17	Mechanism of ligand recognition by human ACE2 receptor **2020**,		2
16	Pathways and Mechanism of Caffeine Binding to Human Adenosine A Receptor. *Frontiers in Molecular Biosciences*, **2021**, 8, 673170	5.6	2
15	Recognition of single-stranded nucleic acids by small-molecule splicing modulators. *Nucleic Acids Research*, **2021**, 49, 7870-7883	20.1	2

14	Docking simulation and antibiotic discovery targeting the MlaC protein in Gram-negative bacteria. *Chemical Biology and Drug Design*, **2019**, 93, 647-652	2.9	2
13	Ligand Gaussian accelerated molecular dynamics (LiGaMD): Characterization of ligand binding thermodynamics and kinetics		1
12	G-Protein-Coupled Receptor-Membrane Interactions Depend on the Receptor Activation state		1
11	Retrospective Ensemble Docking of Allosteric Modulators in an Adenosine G-Protein-Coupled Receptor		1
10	Mechanism of RNA recognition by a Musashi RNA-binding protein		1
9	Efficient purification and assembly of ribonucleoprotein complex for interaction analysis by MST assay coupled with GaMD simulations. *STAR Protocols*, **2021**, 2, 100315	1.4	1
8	Hybrid finite element and Brownian dynamics method for charged particles. *Journal of Chemical Physics*, **2016**, 144, 164107	3.9	1
7	Specific Engineered G Protein Coupling to Histamine Receptors Revealed from Cellular Assay Experiments and Accelerated Molecular Dynamics Simulations. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
6	Structure and mechanism of the γ-secretase intramembrane protease complex.. *Current Opinion in Structural Biology*, **2022**, 74, 102373	8.1	1
5	Molecular Simulations and Drug Discovery of Adenosine Receptors.. *Molecules*, **2022**, 27,	4.8	1
4	Mechanism of Peptide Agonist Binding in CXCR4 Chemokine Receptor.. *Frontiers in Molecular Biosciences*, **2022**, 9, 821055	5.6	0
3	Mechanism of tethered agonist-mediated signaling by polycystin-1.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2113786119	11.5	0
2	Activation of the M2 Muscarinic Receptor and Computer-Aided Design of Receptor-Selective Allosteric Drugs. *Biophysical Journal*, **2014**, 106, 101a	2.9	
1	Temperature Dependent Dynamics of Cytochrome P450cam from Elastic Incoherent Neutron Scattering. *Biophysical Journal*, **2012**, 102, 382a	2.9	