Chia-En A Chang

List of Publications by Year
in descending order

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Version: 2024-02-01

82 papers	3,405 citations	159525 30 h-index	149623 56 g-index
89 all docs	89 docs citations	89 times ranked	4322 citing authors

#	Article	IF	Citations
1	Ligand configurational entropy and protein binding. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 1534-1539.	3.3	350
2	Calculation of Cyclodextrin Binding Affinities: Energy, Entropy, and Implications for Drug Design. Biophysical Journal, 2004, 87, 3035-3049.	0.2	217
3	Free Energy, Entropy, and Induced Fit in Hostâ^'Guest Recognition:Â Calculations with the Second-Generation Mining Minima Algorithm. Journal of the American Chemical Society, 2004, 126, 13156-13164.	6.6	211
4	Evaluating the Accuracy of the Quasiharmonic Approximation. Journal of Chemical Theory and Computation, 2005, 1, 1017-1028.	2.3	160
5	Endosidin2 targets conserved exocyst complex subunit EXO70 to inhibit exocytosis. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E41-50.	3.3	129
6	Flap opening dynamics in HIV-1 protease explored with a coarse-grained model. Journal of Structural Biology, 2007, 157, 606-615.	1.3	113
7	Structural basis for selective activation of ABA receptors. Nature Structural and Molecular Biology, 2010, 17, 1109-1113.	3.6	104
8	Tork: Conformational analysis method for molecules and complexes. Journal of Computational Chemistry, 2003, 24, 1987-1998.	1.5	102
9	X-ray and NMR Crystallography in an Enzyme Active Site: The Indoline Quinonoid Intermediate in Tryptophan Synthase. Journal of the American Chemical Society, 2011, 133, 4-7.	6.6	101
10	The Influence of Macromolecular Crowding on HIV-1 Protease Internal Dynamics. Journal of the American Chemical Society, 2006, 128, 6006-6007.	6.6	96
11	Potential Mean Force from Umbrella Sampling Simulations: What Can We Learn and What Is Missed?. Journal of Chemical Theory and Computation, 2019, 15, 2433-2443.	2.3	96
12	Gated Binding of Ligands to HIV-1 Protease: Brownian Dynamics Simulations in a Coarse-Grained Model. Biophysical Journal, 2006, 90, 3880-3885.	0.2	80
13	Calculation of Molecular Configuration Integrals. Journal of Physical Chemistry B, 2003, 107, 1048-1055.	1.2	76
14	HIV-1 Protease Substrate Binding and Product Release Pathways Explored with Coarse-Grained Molecular Dynamics. Biophysical Journal, 2007, 92, 4179-4187.	0.2	74
15	Entropic contributions and the influence of the hydrophobic environment in promiscuous proteinâ€"protein association. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 7456-7461.	3.3	69
16	ARGONAUTE PIWI domain and microRNA duplex structure regulate small RNA sorting in Arabidopsis. Nature Communications, 2014, 5, 5468.	5.8	69
17	Binding Pathways of Ligands to HIV-1 Protease: Coarse-grained and Atomistic Simulations. Chemical Biology and Drug Design, 2007, 69, 5-13.	1.5	67
18	Heterogeneous CPU+GPU-Enabled Simulations for DFTB Molecular Dynamics of Large Chemical and Biological Systems. Journal of Chemical Theory and Computation, 2019, 15, 2807-2815.	2.3	65

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19	Tuning Enzyme Kinetics through Designed Intermolecular Interactions Far from the Active Site. ACS Catalysis, 2015, 5, 2149-2153.	5.5	61
20	Protonation States of the Tryptophan Synthase Internal Aldimine Active Site from Solid-State NMR Spectroscopy: Direct Observation of the Protonated Schiff Base Linkage to Pyridoxal-5â€²-Phosphate. Journal of the American Chemical Society, 2014, 136, 12824-12827.	6.6	52
21	Ligand Binding Pathways and Conformational Transitions of the HIV Protease. Biochemistry, 2018, 57, 1533-1541.	1.2	52
22	Insights Into Dynamics of Inhibitor and Ubiquitin-Like Protein Binding in SARS-CoV-2 Papain-Like Protease. Frontiers in Molecular Biosciences, 2020, 7, 174.	1.6	51
23	The Entropic Cost of Protein-Protein Association: A Case Study on Acetylcholinesterase Binding to Fasciculin-2. Biophysical Journal, 2005, 89, L25-L27.	0.2	44
24	Binding Thermodynamics and Kinetics Calculations Using Chemical Host and Guest: A Comprehensive Picture of Molecular Recognition. Journal of Chemical Theory and Computation, 2018, 14, 303-318.	2.3	42
25	Amino Acid Networks in a (Î²/Î±)₈ Barrel Enzyme Change during Catalytic Turnover. Journal of the American Chemical Society, 2014, 136, 6818-6821.	6.6	41
26	The Role of Oligomerization and Cooperative Regulation in Protein Function: The Case of Tryptophan Synthase. PLoS Computational Biology, 2010, 6, e1000994.	1.5	40
27	Concepts in Receptor Optimization:Â Targeting the RGD Peptide. Journal of the American Chemical Society, 2006, 128, 4675-4684.	6.6	39
28	Modeling of Enhanced Catalysis in Multienzyme Nanostructures: Effect of Molecular Scaffolds, Spatial Organization, and Concentration. Journal of Chemical Theory and Computation, 2015, 11, 286-292.	2.3	37
29	Gating and Intermolecular Interactions in Ligand-Protein Association: Coarse-Grained Modeling of HIV-1 Protease. Journal of Chemical Theory and Computation, 2011, 7, 3438-3446.	2.3	36
30	Mechanisms of Enhanced Catalysis in Enzymeâ€“DNA Nanostructures Revealed through Molecular Simulations and Experimental Analysis. ChemBioChem, 2016, 17, 1430-1436.	1.3	35
31	Insights from Free-Energy Calculations: Protein Conformational Equilibrium, Driving Forces, and Ligand-Binding Modes. Biophysical Journal, 2012, 103, 342-351.	0.2	30
32	Mechanism of the Association Pathways for a Pair of Fast and Slow Binding Ligands of HIV-1 Protease. Biochemistry, 2017, 56, 1311-1323.	1.2	30
33	T-Analyst: a program for efficient analysis of protein conformational changes by torsion angles. Journal of Computer-Aided Molecular Design, 2010, 24, 819-827.	1.3	29
34	Dynamics of the Acetylcholinesterase Tetramer. Biophysical Journal, 2008, 94, 1144-1154.	0.2	28
35	Visualizing the tunnel in tryptophan synthase with crystallography: Insights into a selective filter for accommodating indole and rejecting water. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2016, 1864, 268-279.	1.1	26
36	Structure and noncanonical Cdk8 activation mechanism within an Argonaute-containing Mediator kinase module. Science Advances, 2021, 7, .	4.7	26

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37	Diffusional Channeling in the Sulfate-Activating Complex: Combined Continuum Modeling and Coarse-Grained Brownian Dynamics Studies. Biophysical Journal, 2008, 95, 4659-4667.	0.2	25
38	Synergistic Regulation and Ligand-Induced Conformational Changes of Tryptophan Synthase. Biochemistry, 2009, 48, 9921-9931.	1.2	25
39	Thermal Isomerization of Cannabinoid Analogues. Journal of the American Chemical Society, 2009, 131, 16640-16641.	6.6	24
40	Protonation states and catalysis: Molecular dynamics studies of intermediates in tryptophan synthase. Protein Science, 2016, 25, 166-183.	3.1	23
41	Switches of hydrogen bonds during ligandâ€“protein association processes determine binding kinetics. Journal of Molecular Recognition, 2014, 27, 537-548.	1.1	21
42	Characterization of Promiscuous Binding of Phosphor Ligands to Breast-Cancer-Gene 1 (BRCA1) C-Terminal (BRCT): Molecular Dynamics, Free Energy, Entropy and Inhibitor Design. PLoS Computational Biology, 2016, 12, e1005057.	1.5	21
43	Role of Molecular Interactions and Protein Rearrangement in the Dissociation Kinetics of p38Î± MAP Kinase Type-I/II/III Inhibitors. Journal of Chemical Information and Modeling, 2018, 58, 968-981.	2.5	19
44	Transient States and Barriers from Molecular Simulations and the Milestoning Theory: Kinetics in Ligandâ€“Protein Recognition and Compound Design. Journal of Chemical Theory and Computation, 2020, 16, 1882-1895.	2.3	19
45	Adaptation of a Genetic Screen Reveals an Inhibitor for Mitochondrial Protein Import Component Tim44. Journal of Biological Chemistry, 2017, 292, 5429-5442.	1.6	18
46	Understanding ligand-receptor non-covalent binding kinetics using molecular modeling. Frontiers in Bioscience - Landmark, 2017, 22, 960-981.	3.0	18
47	Imaging active site chemistry and protonation states: NMR crystallography of the tryptophan synthase Î±-aminoacrylate intermediate. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	18
48	The paradox of conformational constraint in the design of Cbl(TKB)-binding peptides. Scientific Reports, 2013, 3, 1639.	1.6	17
49	Construction of a Sequenceable Protein Mimetic Peptide Library with a True 3D Diversifiable Chemical Space. Journal of the American Chemical Society, 2018, 140, 14552-14556.	6.6	16
50	Inhibiting Matrix Metalloproteinase-2 Activation by Perturbing Proteinâ€“Protein Interactions Using a Cyclic Peptide. Journal of Medicinal Chemistry, 2020, 63, 6979-6990.	2.9	16
51	Ligand-specific homology modeling of human cannabinoid (CB1) receptor. Journal of Molecular Graphics and Modelling, 2012, 38, 155-164.	1.3	14
52	Facet Selectivity of Ligands on Silver Nanoplates: Molecular Mechanics Study. Journal of Physical Chemistry C, 2014, 118, 21589-21598.	1.5	14
53	Syrbactin Structural Analog TIR-199 Blocks Proteasome Activity and Induces Tumor Cell Death. Journal of Biological Chemistry, 2016, 291, 8350-8362.	1.6	14
54	Dynamics and molecular interactions of single-stranded DNA in nucleic acid biosensors with varied surface properties. Physical Chemistry Chemical Physics, 2019, 21, 16367-16380.	1.3	13

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55	Mechanism of PhosphoThreonine/Serine Recognition and Specificity for Modular Domains from All-atom Molecular Dynamics. BMC Biophysics, 2011, 4, 12.	4.4	12
56	Protein binding for detection of small changes on a nanoparticle surface. Analyst, The, 2014, 139, 1364-1371.	1.7	12
57	Investigation of Structural Dynamics of Enzymes and Protonation States of Substrates Using Computational Tools. Catalysts, 2016, 6, 82.	1.6	12
58	A molecular dynamics investigation of CDK8/CycC and ligand binding: conformational flexibility and implication in drug discovery. Journal of Computer-Aided Molecular Design, 2018, 32, 671-685.	1.3	12
59	Agonist and antagonist binding to the nuclear vitamin D receptor: dynamics, mutation effects and functional implications. In Silico Pharmacology, 2013, 1, 2.	1.8	11
60	Analysis of Ligandâ€“Receptor Association and Intermediate Transfer Rates in Multienzyme Nanostructures with All-Atom Brownian Dynamics Simulations. Journal of Physical Chemistry B, 2016, 120, 8518-8531.	1.2	11
61	Discovery of antimicrobial agent targeting tryptophan synthase. Protein Science, 2022, 31, 432-442.	3.1	10
62	Coordinated Network Changes across the Catalytic Cycle of Alpha Tryptophan Synthase. Structure, 2019, 27, 1405-1415.e5.	1.6	9
63	Homology Modeling of Cannabinoid Receptors: Discovery of Cannabinoid Analogues for Therapeutic Use. Methods in Molecular Biology, 2012, 819, 595-613.	0.4	8
64	Immunoproteasome inhibition and bioactivity of thiasyrbactins. Bioorganic and Medicinal Chemistry, 2018, 26, 401-412.	1.4	8
65	Discovery of CDK8/CycC Ligands with a New Virtual Screening Tool. ChemMedChem, 2019, 14, 107-118.	1.6	8
66	Systematic Dissociation Pathway Searches Guided by Principal Component Modes. Journal of Chemical Theory and Computation, 2017, 13, 2230-2244.	2.3	7
67	Amyloid-Î² (AÎ²42) Peptide Aggregation Rate and Mechanism on Surfaces with Widely Varied Properties: Insights from Brownian Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 5549-5558.	1.2	7
68	Substitution of a Surface-Exposed Residue Involved in an Allosteric Network Enhances Tryptophan Synthase Function in Cells. Frontiers in Molecular Biosciences, 2021, 8, 679915.	1.6	7
69	Exploring the binding properties and structural stability of an opsin in the chytridSpizellomyces punctatususing comparative and molecular modeling. PeerJ, 2017, 5, e3206.	0.9	7
70	Mechanistic Insights into Phosphopeptideâ€“BRCT Domain Association: Preorganization, Flexibility, and Phosphate Recognition. Journal of Physical Chemistry B, 2012, 116, 10247-10258.	1.2	6
71	Modeling Effects of Surface Properties and Probe Density for Nanoscale Biosensor Design: A Case Study of DNA Hybridization near Surfaces. Journal of Physical Chemistry B, 2021, 125, 1746-1754.	1.2	6
72	An MM and QM Study of Biomimetic Catalysis of Diels-Alder Reactions Using Cyclodextrins. Catalysts, 2018, 8, 51.	1.6	5

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73	Ligand Binding Pathway Elucidation for Cryptophane Hostâ€“Guest Complexes. Journal of Chemical Theory and Computation, 2013, 9, 2010-2019.	2.3	4
74	Achieving Peptide Binding Specificity and Promiscuity by Loops: Case of the Forkhead-Associated Domain. PLoS ONE, 2014, 9, e98291.	1.1	4
75	Proteome-Wide Characterizations of N⁶-Methyl-Adenosine Triphosphate- and N⁶-Furfuryl-Adenosine Triphosphate-Binding Capabilities of Kinases. Analytical Chemistry, 2021, 93, 13251-13259.	3.2	4
76	Ritonavir and xk263 Binding-Unbinding with HIV-1 Protease: Pathways, Energy and Comparison. Life, 2022, 12, 116.	1.1	4
77	Molecular Mechanics Study of Flow and Surface Influence in Ligandâ€“Protein Association. Frontiers in Molecular Biosciences, 2021, 8, 659687.	1.6	3
78	Modeling structural interconversion in Alzheimersâ€™ amyloid beta peptide with classical and intrinsically disordered protein force fields. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10005-10022.	2.0	2
79	An Integrated Pharmacological, Structural, and Genetic Analysis of Extracellular Versus Intracellular ROS Production in Neutrophils. Journal of Molecular Biology, 2022, 434, 167533.	2.0	2
80	Atomistic Modelling of Phosphopeptide Recognition for Modular Domains. Annual Reports in Computational Chemistry, 2013, 9, 61-84.	0.9	1
81	Tuning Free Energy by Backbone Conformational Entropy: A Strategy from Disordered Proteins. Biophysical Journal, 2018, 114, 2757-2758.	0.2	1
82	GeomBD3: Brownian Dynamics Simulation Software for Biological and Engineered Systems. Journal of Chemical Information and Modeling, 2022, 62, 2257-2263.	2.5	1