Chun Wu

List of Publications by Year
in descending order

87 papers	7,826 citations	109321 35 h-index	53230 85 g-index
87 all docs	87 docs citations	87 times ranked	9972 citing authors

#	Article	IF	Citations
1	A point-charge force field for molecular mechanics simulations of proteins based on condensed-phase quantum mechanical calculations. Journal of Computational Chemistry, 2003, 24, 1999-2012.	3.3	4,028
2	Folding free-energy landscape of villin headpiece subdomain from molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 4925-4930.	7.1	217
3	Human Islet Amyloid Polypeptide Monomers Form Ordered Î²-hairpins: A Possible Direct Amyloidogenic Precursor. Journal of the American Chemical Society, 2009, 131, 18283-18292.	13.7	204
4	The Amyloid Formation Mechanism in Human IAPP: Dimers Have Î²-Strand Monomerâ^'Monomer Interfaces. Journal of the American Chemical Society, 2011, 133, 7240-7243.	13.7	195
5	Coarse-grained models for protein aggregation. Current Opinion in Structural Biology, 2011, 21, 209-220.	5.7	170
6	Dual Binding Modes of Congo Red to Amyloid Protofibril Surface Observed in Molecular Dynamics Simulations. Journal of the American Chemical Society, 2007, 129, 1225-1232.	13.7	163
7	Strike a balance: Optimization of backbone torsion parameters of AMBER polarizable force field for simulations of proteins and peptides. Journal of Computational Chemistry, 2006, 27, 781-790.	3.3	159
8	Binding of Congo Red to Amyloid Protofibrils of the Alzheimer AÎ²9â€“40 Peptide Probed by Molecular Dynamics Simulations. Biophysical Journal, 2012, 103, 550-557.	0.5	140
9	The Binding of Thioflavin T and Its Neutral Analog BTA-1 to Protofibrils of the Alzheimerâ€™s Disease AÎ²16â€“22 Peptide Probed by Molecular Dynamics Simulations. Journal of Molecular Biology, 2008, 384, 718-729.	4.2	132
10	Binding Modes of Thioflavin-T to the Single-Layer Î²-Sheet of the Peptide Self-Assembly Mimics. Journal of Molecular Biology, 2009, 394, 627-633.	4.2	120
11	Convergence of replica exchange molecular dynamics. Journal of Chemical Physics, 2005, 123, 154105.	3.0	107
12	The Structure of AÎ²42 C-Terminal Fragments Probed by a Combined Experimental and Theoretical Study. Journal of Molecular Biology, 2009, 387, 492-501.	4.2	84
13	On the Origin of the Stronger Binding of PIB over Thioflavin T to Protofibrils of the Alzheimer Amyloid-Î² Peptide: A Molecular Dynamics Study. Biophysical Journal, 2011, 100, 1316-1324.	0.5	83
14	Ion Mobility Spectrometry Reveals the Mechanism of Amyloid Formation of AÎ²(25â€“35) and Its Modulation by Inhibitors at the Molecular Level: Epigallocatechin Gallate and Scyllo-inositol. Journal of the American Chemical Society, 2013, 135, 16926-16937.	13.7	83
15	Structural Similarities and Differences between Amyloidogenic and Non-Amyloidogenic Islet Amyloid Polypeptide (IAPP) Sequences and Implications for the Dual Physiological and Pathological Activities of These Peptides. PLoS Computational Biology, 2013, 9, e1003211.	3.2	78
16	Elongation of Ordered Peptide Aggregate of an Amyloidogenic Hexapeptide NFGAIL Observed in Molecular Dynamics Simulations with Explicit Solvent. Journal of the American Chemical Society, 2005, 127, 13530-13537.	13.7	77
17	Surface force measurements and simulations of mussel-derived peptide adhesives on wet organic surfaces. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4332-4337.	7.1	77
18	AÎ²(39â€“42) Modulates AÎ² Oligomerization but Not Fibril Formation. Biochemistry, 2012, 51, 108-117.	2.5	72

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19	Development and Characterization of Monoclonal Antibodies Specific to the Serotonin 5-HT_{2A}Receptor. Journal of Histochemistry and Cytochemistry, 1998, 46, 811-824.	2.5	68
20	Oligomers of the Prion Protein Fragment 106â˜'126 Are Likely Assembled from Î²-Hairpins in Solution, and Methionine Oxidation Inhibits Assembly without Altering the Peptideâ€™s Monomeric Conformation. Journal of the American Chemical Society, 2010, 132, 532-539.	13.7	67
21	Defining the Molecular Basis of Amyloid Inhibitors: Human Islet Amyloid Polypeptideâ€“Insulin Interactions. Journal of the American Chemical Society, 2014, 136, 12912-12919.	13.7	67
22	Phenol Red Interacts with the Protofibril-Like Oligomers of an Amyloidogenic Hexapeptide NFGAIL through Both Hydrophobic and Aromatic Contacts. Biophysical Journal, 2006, 91, 3664-3672.	0.5	61
23	The Role of Phe in the Formation of Well-Ordered Oligomers of Amyloidogenic Hexapeptide (NFGAIL) Observed in Molecular Dynamics Simulations with Explicit Solvent. Biophysical Journal, 2005, 88, 2897-2906.	0.5	60
24	Analysis of the Amyloidogenic Potential of Pufferfish (Takifugu rubripes) Islet Amyloid Polypeptide Highlights the Limitations of Thioflavin-T Assays and the Difficulties in Defining Amyloidogenicity. Biochemistry, 2016, 55, 510-518.	2.5	59
25	Formation of Partially Ordered Oligomers of Amyloidogenic Hexapeptide (NFGAIL) in Aqueous Solution Observed in Molecular Dynamics Simulations. Biophysical Journal, 2004, 87, 3000-3009.	0.5	57
26	Breaking non-native hydrophobic clusters is the rate-limiting step in the folding of an alanine-based peptide. Biopolymers, 2003, 68, 63-75.	2.4	55
27	Molecular Structures of Quiescently Grown and Brain-Derived Polymorphic Fibrils of the Alzheimer Amyloid AÎ²9-40 Peptide: A Comparison to Agitated Fibrils. PLoS Computational Biology, 2010, 6, e1000693.	3.2	54
28	Early stage intercalation of doxorubicin to DNA fragments observed in molecular dynamics binding simulations. Journal of Molecular Graphics and Modelling, 2012, 38, 279-289.	2.4	52
29	Mechanism of C-Terminal Fragments of Amyloid Î²-Protein as AÎ² Inhibitors: Do C-Terminal Interactions Play a Key Role in Their Inhibitory Activity?. Journal of Physical Chemistry B, 2016, 120, 1615-1623.	2.6	47
30	Discovery and optimization of 1-(1 H -indol-1-yl)ethanone derivatives as CBP/EP300 bromodomain inhibitors for the treatment of castration-resistant prostate cancer. European Journal of Medicinal Chemistry, 2018, 147, 238-252.	5.5	46
31	Structure-Based Discovery and Optimization of Benzo[d]isoxazole Derivatives as Potent and Selective BET Inhibitors for Potential Treatment of Castration-Resistant Prostate Cancer (CRPC). Journal of Medicinal Chemistry, 2018, 61, 3037-3058.	6.4	46
32	Assessing the Performance of Popular Quantum Mechanics and Molecular Mechanics Methods and Revealing the Sequence-Dependent Energetic Features Using 100 Tetrapeptide Models. Journal of Chemical Theory and Computation, 2010, 6, 1199-1209.	5.3	42
33	Binding of BRACO19 to a Telomeric G-Quadruplex DNA Probed by All-Atom Molecular Dynamics Simulations with Explicit Solvent. Molecules, 2019, 24, 1010.	3.8	42
34	Probing the Binding Pathway of BRACO19 to a Parallel-Stranded Human Telomeric G-Quadruplex Using Molecular Dynamics Binding Simulation with AMBER DNA OL15 and Ligand GAFF2 Force Fields. Journal of Chemical Information and Modeling, 2017, 57, 2846-2864.	5.4	40
35	Computational and Experimental Analyses Reveal the Essential Roles of Interdomain Linkers in the Biological Function of Chemotaxis Histidine Kinase CheA. Journal of the American Chemical Society, 2012, 134, 16107-16110.	13.7	36
36	The Linker between the Dimerization and Catalytic Domains of the CheA Histidine Kinase Propagates Changes in Structure and Dynamics That Are Important for Enzymatic Activity. Biochemistry, 2014, 53, 855-861.	2.5	36

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37	Accurate ab Initio Study on the Hydrogen-Bond Pairs in Protein Secondary Structures. Journal of Chemical Theory and Computation, 2007, 3, 1527-1537.	5.3	35
38	Folding processes of the B domain of protein A to the native state observed in all-atom ab initio folding simulations. Journal of Chemical Physics, 2008, 128, 235105.	3.0	35
39	Binding of Telomestatin, TMPyP4, BSU6037, and BRACO19 to a Telomeric G-Quadruplexâ€“Duplex Hybrid Probed by All-Atom Molecular Dynamics Simulations with Explicit Solvent. ACS Omega, 2018, 3, 14788-14806.	3.5	32
40	Mechanistic insight on the remdesivir binding to RNA-Dependent RNA polymerase (RdRp) of SARS-cov-2. Computers in Biology and Medicine, 2021, 129, 104156.	7.0	31
41	Strictinin, a novel ROR1-inhibitor, represses triple negative breast cancer survival and migration via modulation of PI3K/AKT/GSK3ÃŸ activity. PLoS ONE, 2019, 14, e0217789.	2.5	30
42	Molecular Dynamics Simulations and Free Energy Analyses on the Dimer Formation of an Amyloidogenic Heptapeptide from Human Î²2-Microglobulin: Implication for the Protofibril Structure. Journal of Molecular Biology, 2006, 356, 1049-1063.	4.2	28
43	Hetero-oligomeric Amyloid Assembly and Mechanism: Prion Fragment PrP(106â€“126) Catalyzes the Islet Amyloid Polypeptide Î²-Hairpin. Journal of the American Chemical Society, 2018, 140, 9685-9695.	13.7	28
44	Binding of Telomestatin to a Telomeric G-Quadruplex DNA Probed by All-Atom Molecular Dynamics Simulations with Explicit Solvent. Journal of Chemical Information and Modeling, 2016, 56, 2093-2102.	5.4	26
45	Binding modes and pathway of RHPS4 to human telomeric G-quadruplex and duplex DNA probed by all-atom molecular dynamics simulations with explicit solvent. Physical Chemistry Chemical Physics, 2017, 19, 18685-18694.	2.8	26
46	Development of a novel series of non-natural triaryl agonists and antagonists of the Pseudomonas aeruginosa LasR quorum sensing receptor. Bioorganic and Medicinal Chemistry, 2017, 25, 153-165.	3.0	25
47	Dual folding pathways of an Î±/Î² protein from all-atom ab initio folding simulations. Journal of Chemical Physics, 2009, 131, 165105.	3.0	22
48	Dopamine D₄ Receptor-Selective Compounds Reveal Structureâ€“Activity Relationships that Engender Agonist Efficacy. Journal of Medicinal Chemistry, 2019, 62, 3722-3740.	6.4	20
49	Drug repurposing against SARS-CoV-2 receptor binding domain using ensemble-based virtual screening and molecular dynamics simulations. Computers in Biology and Medicine, 2021, 135, 104634.	7.0	20
50	Binding of anticancer drug daunomycin to a TGGGGT G-quadruplex DNA probed by all-atom molecular dynamics simulations: additional pure groove binding mode and implications on designing more selective G-quadruplex ligands. Journal of Molecular Modeling, 2017, 23, 256.	1.8	19
51	Elucidation of partial activation of cannabinoid receptor type 2 and identification of potential partial agonists: Molecular dynamics simulation and structure-based virtual screening. Computational Biology and Chemistry, 2022, 99, 107723.	2.3	19
52	On the Origins of the Weak Folding Cooperativity of a Designed Î²Î²Î± Ultrafast Protein FSD-1. PLoS Computational Biology, 2010, 6, e1000998.	3.2	14
53	How accurate are the popular PCM/GB continuum solvation models for calculating the solvation energies of amino acid side-chain analogs?. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	14
54	Computational analysis of Amsacrine resistance in human topoisomerase II alpha mutants (R487K and) Tj ETQq0 0 0 rgBT /Overlock 10 T solvent. Journal of Molecular Graphics and Modelling, 2017, 72, 209-219.	2.4	14

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55	Y08060: A Selective BET Inhibitor for Treatment of Prostate Cancer. ACS Medicinal Chemistry Letters, 2018, 9, 262-267.	2.8	14
56	To probe interaction of morphine and IBNtxA with 7TM and 6TM variants of the human Î¼-opioid receptor using all-atom molecular dynamics simulations with an explicit membrane. Physical Chemistry Chemical Physics, 2018, 20, 1724-1741.	2.8	14
57	Effects of Ionic Liquids on Metalloproteins. Molecules, 2021, 26, 514.	3.8	14
58	Rapid simultaneous determination of four anthracene derivatives using a single non-linear variable-angle synchronous fluorescence spectrum. Fresenius' Journal of Analytical Chemistry, 2000, 368, 669-675.	1.5	13
59	Three-Dimensional Structure of RNA Monomeric G-Quadruplex Containing ALS and FTD Related G4C2 Repeat and Its Binding with TMPyP4 Probed by Homology Modeling based on Experimental Constraints and Molecular Dynamics Simulations. ACS Chemical Neuroscience, 2020, 11, 57-75.	3.5	13
60	Probing biased activation of mu-opioid receptor by the biased agonist PZM21 using all atom molecular dynamics simulation. Life Sciences, 2021, 269, 119026.	4.3	13
61	Molecular Dynamics Study on the Binding of an Anticancer DNA G-Quadruplex Stabilizer, CX-5461, to Human Telomeric, c-KIT1, and c-Myc G-Quadruplexes and a DNA Duplex. Journal of Chemical Information and Modeling, 2020, 60, 5203-5224.	5.4	12
62	Computational Study of Anticancer Drug Resistance Caused by 10 Topisomerase I Mutations, Including 7 Camptothecin Analogs and Lucanthone. Journal of Chemical Information and Modeling, 2016, 56, 1872-1883.	5.4	11
63	An Experimental and Molecular Dynamics Study of Red Fluorescent Protein mCherry in Novel Aqueous Amino Acid Ionic Liquids. Journal of Physical Chemistry B, 2017, 121, 4823-4832.	2.6	11
64	Computational insights into differential interaction of mammalian angiotensin-converting enzyme 2 with the SARS-CoV-2 spike receptor binding domain. Computers in Biology and Medicine, 2022, 141, 105017.	7.0	11
65	Molecular dynamics simulation of biased agonists at the dopamine D2 receptor suggests the mechanism of receptor functional selectivity. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3206-3225.	3.5	9
66	Novel inhibitors to ADP ribose phosphatase of SARS-CoV-2 identified by structure-based high throughput virtual screening and molecular dynamics simulations. Computers in Biology and Medicine, 2022, 140, 105084.	7.0	9
67	Derivative Matrix Isopotential Synchronous Fluorescence Spectroscopy for the Direct Determination of 1-Hydroxypyrene as a Urinary Biomarker of Exposure to Polycyclic Aromatic Hydrocarbons.. Analytical Sciences, 2001, 17, 167-170.	1.6	8
68	Experimental and Simulation Identification of Xanthohumol as an Inhibitor and Substrate of ABCB1. Applied Sciences (Switzerland), 2018, 8, 681.	2.5	8
69	GDP Release from the Open Conformation of GÎ± Requires Allosteric Signaling from the Agonist-Bound Human Î²₂ Adrenergic Receptor. Journal of Chemical Information and Modeling, 2020, 60, 4064-4075.	5.4	8
70	Binding Interactions of Ergotamine and Dihydroergotamine to 5-Hydroxytryptamine Receptor 1B (5-HT_{1b}) Using Molecular Dynamics Simulations and Dynamic Network Analysis. Journal of Chemical Information and Modeling, 2020, 60, 1749-1765.	5.4	8
71	To Probe Full and Partial Activation of Human Peroxisome Proliferator-Activated Receptors by Pan-Agonist Chiglitazar Using Molecular Dynamics Simulations. PPAR Research, 2020, 2020, 1-24.	2.4	8
72	Binding of agonist WAY-267,464 and antagonist WAY-methylated to oxytocin receptor probed by all-atom molecular dynamics simulations. Life Sciences, 2020, 252, 117643.	4.3	8

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73	Activation Mechanism of Corticotrophin Releasing Factor Receptor Type 1 Elucidated Using Molecular Dynamics Simulations. ACS Chemical Neuroscience, 2021, 12, 1674-1687.	3.5	8
74	The Structure of Intrinsically Disordered Peptides Implicated in Amyloid Diseases: Insights from Fully Atomistic Simulations. Biological and Medical Physics Series, 2012, , 215-227.	0.4	8
75	Can human allergy drug fexofenadine, an antagonist of histamine (H1) receptor, be used to treat dog and cat? Homology modeling, docking and molecular dynamic Simulation of three H1 receptors in complex with fexofenadine. Journal of Molecular Graphics and Modelling, 2017, 75, 106-116.	2.4	7
76	Analysis of vismodegib resistance in D473G and W535L mutants of SMO receptor and design of novel drug derivatives using molecular dynamics simulations. Life Sciences, 2020, 244, 117302.	4.3	7
77	Thermodynamic destabilization of azurin by four different tetramethylguanidinium amino acid ionic liquids. International Journal of Biological Macromolecules, 2021, 180, 355-364.	7.5	7
78	To Probe the Binding Interactions between Two FDA Approved Migraine Drugs (Ubrogepant and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 5 Simulations. ACS Chemical Neuroscience, 2021, 12, 2629-2642.	3.5	7
79	Interaction analyses of hTAAR1 and mTAAR1 with antagonist EPPTB. Life Sciences, 2022, 300, 120553.	4.3	6
80	To probe the binding pathway of a selective compound (D089-0563) to c-MYC Pu24 G-quadruplex using free ligand binding simulations and Markov state model analysis. Physical Chemistry Chemical Physics, 2020, 22, 22567-22583.	2.8	5
81	Investigating detailed interactions between novel PAR1 antagonist F16357 and the receptor using docking and molecular dynamic simulations. Journal of Molecular Graphics and Modelling, 2017, 77, 205-217.	2.4	4
82	QM/MM MD simulations reveal an asynchronous PCET mechanism for nitrite reduction by copper nitrite reductase. Physical Chemistry Chemical Physics, 2020, 22, 20922-20928.	2.8	4
83	Unraveling the binding mechanism of the active form of Remdesivir to RdRp of SARS-CoV-2 and designing new potential analogues: Insights from molecular dynamics simulations. Chemical Physics Letters, 2022, 799, 139638.	2.6	4
84	Y06014 is a selective BET inhibitor for the treatment of prostate cancer. Acta Pharmacologica Sinica, 2021, 42, 2120-2131.	6.1	3
85	Effects of Ionic Liquids on Laccase from Trametes versicolor. Biophysica, 2021, 1, 429-444.	1.4	2
86	Novel Dopamine D4 Receptorâ€Selective Compounds Reveal Structureâ€Activity Relationships that Engender Agonist Efficacy. FASEB Journal, 2019, 33, lb40.	0.5	0
87	Binding of GS-461203 and Its Halogen Derivatives to HCV Genotype 2a RNA Polymerase Drug Resistance Mutants. Scientia Pharmaceutica, 2022, 90, 26.	2.0	0