Jung-Hsin Lin

List of Publications by Year
in descending order

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56 papers	2,661 citations	279798 23 h-index	197818 49 g-index
57 all docs	57 docs citations	57 times ranked	3702 citing authors

#	Article	IF	Citations
1	Computational Drug Design Accommodating Receptor Flexibility:Â The Relaxed Complex Scheme. Journal of the American Chemical Society, 2002, 124, 5632-5633.	13.7	401
2	HIV-1 protease molecular dynamics of a wild-type and of the V82F/I84V mutant: Possible contributions to drug resistance and a potential new target site for drugs. Protein Science, 2004, 13, 1108-1123.	7.6	217
3	Statins Increase p21 through Inhibition of Histone Deacetylase Activity and Release of Promoter-Associated HDAC1/2. Cancer Research, 2008, 68, 2375-2383.	0.9	182
4	The relaxed complex method: Accommodating receptor flexibility for drug design with an improved scoring scheme. Biopolymers, 2003, 68, 47-62.	2.4	175
5	Remarkable Loop Flexibility in Avian Influenza N1 and Its Implications for Antiviral Drug Design. Journal of the American Chemical Society, 2007, 129, 7764-7765.	13.7	157
6	idTarget: a web server for identifying protein targets of small chemical molecules with robust scoring functions and a divide-and-conquer docking approach. Nucleic Acids Research, 2012, 40, W393-W399.	14.5	150
7	Increased Membrane Affinity of the C1 Domain of Protein Kinase CÎ´ Compensates for the Lack of Involvement of Its C2 Domain in Membrane Recruitment. Journal of Biological Chemistry, 2006, 281, 1660-1669.	3.4	112
8	Stability of a Melittin Pore in a Lipid Bilayer: A Molecular Dynamics Study. Biophysical Journal, 2000, 78, 1714-1724.	0.5	101
9	Genetic determinants of antithyroid drug-induced agranulocytosis by human leukocyte antigen genotyping and genome-wide association study. Nature Communications, 2015, 6, 7633.	12.8	93
10	MEDock: a web server for efficient prediction of ligand binding sites based on a novel optimization algorithm. Nucleic Acids Research, 2005, 33, W233-W238.	14.5	92
11	Improvement of porphyrins for G-quadruplex DNA targeting. Biochimie, 2011, 93, 1310-1317.	2.6	76
12	A New Drug Design Targeting the Adenosinergic System for Huntington's Disease. PLoS ONE, 2011, 6, e20934.	2.5	73
13	Bridging Implicit and Explicit Solvent Approaches for Membrane Electrostatics. Biophysical Journal, 2002, 83, 1374-1379.	0.5	66
14	Design and Synthesis of Dual-Action Inhibitors Targeting Histone Deacetylases and 3-Hydroxy-3-methylglutaryl Coenzyme A Reductase for Cancer Treatment. Journal of Medicinal Chemistry, 2013, 56, 3645-3655.	6.4	66
15	Accommodating Protein Flexibility for Structure-Based Drug Design. Current Topics in Medicinal Chemistry, 2011, 11, 171-178.	2.1	60
16	Restrained molecular dynamics simulations of HIV-1 protease: The first step in validating a new target for drug design. Biopolymers, 2006, 82, 272-284.	2.4	52
17	Robust Scoring Functions for Proteinâ€“Ligand Interactions with Quantum Chemical Charge Models. Journal of Chemical Information and Modeling, 2011, 51, 2528-2537.	5.4	47
18	Structural insights into the gating of DNA passage by the topoisomerase II DNA-gate. Nature Communications, 2018, 9, 3085.	12.8	47

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19	Scoring Functions for Prediction of Protein-Ligand Interactions. Current Pharmaceutical Design, 2013, 19, 2174-2182.	1.9	46
20	Preparation of secolycorines against acetylcholinesterase. Bioorganic and Medicinal Chemistry, 2007, 15, 1034-1043.	3.0	38
21	Cobalt(<scp>iii</scp>)porphyrin to target G-quadruplex DNA. Dalton Transactions, 2015, 44, 3701-3707.	3.3	35
22	SLITHER: a web server for generating contiguous conformations of substrate molecules entering into deep active sites of proteins or migrating through channels in membrane transporters. Nucleic Acids Research, 2009, 37, W559-W564.	14.5	32
23	Tetrahydropyran- and Tetrahydrofuran-Containing Diarylheptanoids from Hedychium coronarium Rhizomes. Journal of Natural Products, 2015, 78, 181-187.	3.0	25
24	Optimization and Computational Evaluation of a Series of Potential Active Site Inhibitors of the V82F/I84V Drug-resistant Mutant of HIV-1 Protease: an Application of the Relaxed Complex Method of Structure-based Drug Design. Chemical Biology and Drug Design, 2006, 67, 336-345.	3.2	24
25	When Cytokinin, a Plant Hormone, Meets the Adenosine A2A Receptor: A Novel Neuroprotectant and Lead for Treating Neurodegenerative Disorders?. PLoS ONE, 2012, 7, e38865.	2.5	23
26	Protemot: prediction of protein binding sites with automatically extracted geometrical templates. Nucleic Acids Research, 2006, 34, W303-W309.	14.5	22
27	Design and Synthesis of Novel Dualâ€Action Compounds Targeting the Adenosine A_{2A} Receptor and Adenosine Transporter for Neuroprotection. ChemMedChem, 2011, 6, 1390-1400.	3.2	21
28	A simple electrostatic switch important in the activation of type I protein kinase A by cyclic AMP. Protein Science, 2006, 15, 113-121.	7.6	19
29	Inhibition of histone deacetylase activity is a novel function of the antifolate drug methotrexate. Biochemical and Biophysical Research Communications, 2010, 391, 1396-1399.	2.1	18
30	Delineating Proteinâ€"Protein Curvilinear Dissociation Pathways and Energetics with NaÃ¯ve Multipleâ€Walker Umbrella Sampling Simulations. Journal of Computational Chemistry, 2019, 40, 1652-1663.	3.3	18
31	Molecular Dynamics Simulations of the Rotary Motor F0 under External Electric Fields across the Membrane. Biophysical Journal, 2010, 98, 1009-1017.	0.5	17
32	Quantitative phosphoproteomic analysis identifies the potential therapeutic target EphA2 for overcoming sorafenib resistance in hepatocellular carcinoma cells. Experimental and Molecular Medicine, 2020, 52, 497-513.	7.7	15
33	A newly designed molecule J2326 for Alzheimer's disease disaggregates amyloid fibrils and induces neurite outgrowth. Neuropharmacology, 2015, 92, 146-157.	4.1	13
34	Molecular dynamics simulations of hydrophobic and amphiphatic proteins interacting with a lipid bilayer membrane. Computational and Theoretical Polymer Science, 2000, 10, 97-102.	1.1	12
35	AID downregulation is a novel function of the DNMT inhibitor 5-aza-deoxycytidine. Oncotarget, 2014, 5, 211-223.	1.8	12
36	Review structureâ€•and dynamicsâ€based computational design of anticancer drugs. Biopolymers, 2016, 105, 2-9.	2.4	11

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37	AutoBind: automatic extraction of proteinâ€“ligand-binding affinity data from biological literature. Bioinformatics, 2012, 28, 2162-2168.	4.1	10
38	Discovery of Small Molecules for Fluorescent Detection of Complement Activation Product C3d. Journal of Medicinal Chemistry, 2015, 58, 9535-9545.	6.4	10
39	Effect of statin use on the risk of medically attended acute respiratory illness among influenza vaccinated elderly. Vaccine, 2018, 36, 6133-6137.	3.8	9
40	Adsorption of melittin to a lipid bilayer : A molecular dynamics study. Journal of Molecular Liquids, 2000, 84, 89-98.	4.9	8
41	Discovery of Nâ€Arylalkylâ€3â€hydroxyâ€4â€oxoâ€3,4â€dihydroquinazolinâ€2â€carboxamide Derivatives as HCV NS5B Polymerase Inhibitors. ChemMedChem, 2012, 7, 850-860.	3.2	8
42	Target Prediction of Small Molecules with Information of Key Molecular Interactions. Current Topics in Medicinal Chemistry, 2012, 12, 1903-1910.	2.1	7
43	Drug-Induced Conformational Population Shifts in Topoisomerase-DNA Ternary Complexes. Molecules, 2014, 19, 7415-7428.	3.8	7
44	Recovery of the poisoned topoisomerase II for DNA religation: coordinated motion of the cleavage core revealed with the microsecond atomistic simulation. Nucleic Acids Research, 2015, 43, 6772-6786.	14.5	7
45	ON THE DESIGN OF OPTIMIZATION ALGORITHMS FOR PREDICTION OF MOLECULAR INTERACTIONS. International Journal on Artificial Intelligence Tools, 2010, 19, 267-280.	1.0	3
46	Improved enamine-type addition of dehydroaporphine using microwave irradiation. Tetrahedron Letters, 2010, 51, 3062-3064.	1.4	2
47	A Curvilinear-Path Umbrella Sampling Approach to Characterizing the Interactions Between Rapamycin and Three FKBP12 Variants. Frontiers in Molecular Biosciences, 0, 9, .	3.5	2
48	On the Design of Optimization Algorithms for Prediction of Molecular Interactions. , 2009, , .		1
49	Can Ligands of Different Functional Types Induce Distinct Dynamics in G Protein-Coupled Receptors?. Current Topics in Medicinal Chemistry, 2017, 17, 2370-2380.	2.1	1
50	Scoring Functions for Fragment-Based Drug Discovery. Methods in Molecular Biology, 2015, 1289, 101-115.	0.9	1
51	A New Approach to the Discretization of Multidimensional Scaling. , 0, , .		1
52	Molecular Dynamics Simulations of the Rotary Motor F0 Under External Electric Fields Across the Membrane. Biophysical Journal, 2010, 98, 53a.	0.5	0
53	Mechanical Transmission Between the Î³-Subunit of F1 and the C-Ring of Membrane-Bound FO of ATP Synthase: A Molecular Dynamics Study. Biophysical Journal, 2012, 102, 712a.	0.5	0
54	Ligand-Perturbed Allosteric Communication within the Human A2A Adenosine Receptor. Biophysical Journal, 2013, 104, 171a.	0.5	0

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55	Coordinated Dynamics Orchestrating the DNA Re-Ligation by De-Poisoned Topoisomerase II. Biophysical Journal, 2016, 110, 361a-362a.	0.5	0
56	Dynamical Mechanisms of Allosteric Modulations by Small Molecules on Leukocyte Function-Associated Antigen-1. Biophysical Journal, 2017, 112, 496a-497a.	0.5	0