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	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
2	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
3	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
4	Structural insights into the gating of DNA passage by the topoisomerase II DNA-gate. Nature Communications, 2018, 9, 3085.	12.8	47
5	Dynamical Mechanisms of Allosteric Modulations by Small Molecules on Leukocyte Function-Associated Antigen-1. Biophysical Journal, 2017, 112, 496a-497a.	0.5	0
6	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
7	Coordinated Dynamics Orchestrating the DNA Re-Ligation by De-Poisoned Topoisomerase II. Biophysical Journal, 2016, 110, 361a-362a.	0.5	0
8	Review structureâ€•and dynamicsâ€based computational design of anticancer drugs. Biopolymers, 2016, 105, 2-9.	2.4	11
9	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
10	A newly designed molecule J2326 for Alzheimer's disease disaggregates amyloid fibrils and induces neurite outgrowth. Neuropharmacology, 2015, 92, 146-157.	4.1	13
11	Tetrahydropyran- and Tetrahydrofuran-Containing Diarylheptanoids from Hedychium coronarium Rhizomes. Journal of Natural Products, 2015, 78, 181-187.	3.0	25
12	Cobalt(<scp>iii</scp>)porphyrin to target G-quadruplex DNA. Dalton Transactions, 2015, 44, 3701-3707.	3.3	35
13	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
14	Discovery of Small Molecules for Fluorescent Detection of Complement Activation Product C3d. Journal of Medicinal Chemistry, 2015, 58, 9535-9545.	6.4	10
15	Scoring Functions for Fragment-Based Drug Discovery. Methods in Molecular Biology, 2015, 1289, 101-115.	0.9	1
16	Drug-Induced Conformational Population Shifts in Topoisomerase-DNA Ternary Complexes. Molecules, 2014, 19, 7415-7428.	3.8	7
17	AID downregulation is a novel function of the DNMT inhibitor 5-aza-deoxycytidine. Oncotarget, 2014, 5, 211-223.	1.8	12
18	Ligand-Perturbed Allosteric Communication within the Human A2A Adenosine Receptor. Biophysical Journal, 2013, 104, 171a.	0.5	0

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19	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
20	Scoring Functions for Prediction of Protein-Ligand Interactions. Current Pharmaceutical Design, 2013, 19, 2174-2182.	1.9	46
21	AutoBind: automatic extraction of proteinâ€“ligand-binding affinity data from biological literature. Bioinformatics, 2012, 28, 2162-2168.	4.1	10
22	Target Prediction of Small Molecules with Information of Key Molecular Interactions. Current Topics in Medicinal Chemistry, 2012, 12, 1903-1910.	2.1	7
23	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
24	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
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	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
27	A New Drug Design Targeting the Adenosinergic System for Huntington's Disease. PLoS ONE, 2011, 6, e20934.	2.5	73
28	Improvement of porphyrins for G-quadruplex DNA targeting. Biochimie, 2011, 93, 1310-1317.	2.6	76
29	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
30	Accommodating Protein Flexibility for Structure-Based Drug Design. Current Topics in Medicinal Chemistry, 2011, 11, 171-178.	2.1	60
31	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
32	Improved enamine-type addition of dehydroaporphine using microwave irradiation. Tetrahedron Letters, 2010, 51, 3062-3064.	1.4	2
33	Molecular Dynamics Simulations of the Rotary Motor F0 under External Electric Fields across the Membrane. Biophysical Journal, 2010, 98, 1009-1017.	0.5	17
34	Molecular Dynamics Simulations of the Rotary Motor F0 Under External Electric Fields Across the Membrane. Biophysical Journal, 2010, 98, 53a.	0.5	0
35	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
36	ON THE DESIGN OF OPTIMIZATION ALGORITHMS FOR PREDICTION OF MOLECULAR INTERACTIONS. International Journal on Artificial Intelligence Tools, 2010, 19, 267-280.	1.0	3

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37	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
38	On the Design of Optimization Algorithms for Prediction of Molecular Interactions. , 2009, , .		1
39	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
40	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
41	Preparation of secolycorines against acetylcholinesterase. Bioorganic and Medicinal Chemistry, 2007, 15, 1034-1043.	3.0	38
42	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
43	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
44	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
45	Protemot: prediction of protein binding sites with automatically extracted geometrical templates. Nucleic Acids Research, 2006, 34, W303-W309.	14.5	22
46	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
47	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
48	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
49	The relaxed complex method: Accommodating receptor flexibility for drug design with an improved scoring scheme. Biopolymers, 2003, 68, 47-62.	2.4	175
50	Computational Drug Design Accommodating Receptor Flexibility:Â The Relaxed Complex Scheme. Journal of the American Chemical Society, 2002, 124, 5632-5633.	13.7	401
51	Bridging Implicit and Explicit Solvent Approaches for Membrane Electrostatics. Biophysical Journal, 2002, 83, 1374-1379.	0.5	66
52	Adsorption of melittin to a lipid bilayer : A molecular dynamics study. Journal of Molecular Liquids, 2000, 84, 89-98.	4.9	8
53	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
54	Stability of a Melittin Pore in a Lipid Bilayer: A Molecular Dynamics Study. Biophysical Journal, 2000, 78, 1714-1724.	0.5	101

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55	A New Approach to the Discretization of Multidimensional Scaling. , 0, , .		1
56	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