## Jianping Hu

List of Publications by Year in descending order

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LIANDING HU

#	Article	IF	CITATIONS
1	COVID-19 Docking Server: a meta server for docking small molecules, peptides and antibodies against potential targets of COVID-19. Bioinformatics, 2020, 36, 5109-5111.	4.1	122
2	Long Non-coding RNAs: Emerging Roles in the Immunosuppressive Tumor Microenvironment. Frontiers in Oncology, 2020, 10, 48.	2.8	63
3	MAPKâ€Targeted Drug Delivered by a pHâ€Sensitive MSNP Nanocarrier Synergizes with PDâ€1 Blockade in Melanoma without Tâ€Cell Suppression. Advanced Functional Materials, 2019, 29, 1806916.	14.9	34
4	PD-L1 Nanobody Competitively Inhibits the Formation of the PD-1/PD-L1 Complex: Comparative Molecular Dynamics Simulations. International Journal of Molecular Sciences, 2018, 19, 1984.	4.1	31
5	Difference and Influence of Inactive and Active States of Cannabinoid Receptor Subtype CB2: From Conformation to Drug Discovery. Journal of Chemical Information and Modeling, 2016, 56, 1152-1163.	5.4	26
6	Combination of MAPK inhibition with photothermal therapy synergistically augments the anti-tumor efficacy of immune checkpoint blockade. Journal of Controlled Release, 2021, 332, 194-209.	9.9	25
7	Study on the molecular mechanism of inhibiting HIV-1 integrase by EBR28 peptide via molecular modeling approach. Biophysical Chemistry, 2008, 132, 69-80.	2.8	21
8	Metal binding mediated conformational change of XPA protein:a potential cytotoxic mechanism of nickel in the nucleotide excision repair. Journal of Molecular Modeling, 2016, 22, 156.	1.8	18
9	Study on the interactions between diketo-acid inhibitors and prototype foamy virus integrase-DNA complex via molecular docking and comparative molecular dynamics simulation methods. Journal of Biomolecular Structure and Dynamics, 2013, 31, 734-747.	3.5	17
10	Combined 3D-QSAR, molecular docking, and molecular dynamics study of tacrine derivatives as potential acetylcholinesterase (AChE) inhibitors of Alzheimer's disease. Journal of Molecular Modeling, 2015, 21, 277.	1.8	16
11	Integrin-Src-YAP1 signaling mediates the melanoma acquired resistance to MAPK and PI3K/mTOR dual targeted therapy. Molecular Biomedicine, 2020, 1, 12.	4.4	16
12	Efficient whole-cell catalysis for 5-aminovalerate production from L-lysine by using engineered Escherichia coli with ethanol pretreatment. Scientific Reports, 2020, 10, 990.	3.3	16
13	3D-QSAR, Molecular Docking and Molecular Dynamics Simulation of Pseudomonas aeruginosa LpxC Inhibitors. International Journal of Molecular Sciences, 2017, 18, 761.	4.1	15
14	Inhibition of programmed cell death protein ligand-1 (PD-L1) by benzyl ether derivatives: analyses of conformational change, molecular recognition and binding free energy. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4801-4812.	3.5	15
15	Specifically targeting cancer proliferation and metastasis processes: the development of matriptase inhibitors. Cancer and Metastasis Reviews, 2019, 38, 507-524.	5.9	14
16	3D-QSAR and molecular recognition of <i>Klebsiella pneumoniae</i> NDM-1 inhibitors. Molecular Simulation, 2019, 45, 694-705.	2.0	13
17	Concepts and Application of DNA Origami and DNA Self-Assembly: A Systematic Review. Applied Bionics and Biomechanics, 2021, 2021, 1-15.	1.1	12
18	Omicron-included mutation-induced changes in epitopes of SARS-CoV-2 spike protein and effectiveness assessments of current antibodies. Molecular Biomedicine, 2022, 3, 12.	4.4	12

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19	Molecular Dynamics Simulation of HIVâ€1 Integrase Dimer Complexed with Viral DNA. Chinese Journal of Chemistry, 2010, 28, 33-40.	4.9	11
20	The Evolution of Acquired Resistance to BRAFV600EÂkinase inhibitor Is Sustained by IGF1-Driven Tumor Vascular Remodeling. Journal of Investigative Dermatology, 2022, 142, 445-458.	0.7	11
21	Probing the Behaviour of Cas1-Cas2 upon Protospacer Binding in CRISPR-Cas Systems using Molecular Dynamics Simulations. Scientific Reports, 2019, 9, 3188.	3.3	10
22	Structural characterization of the Plasmodium falciparum lactate transporter PfFNT alone and in complex with antimalarial compound MMV007839 reveals its inhibition mechanism. PLoS Biology, 2021, 19, e3001386.	5.6	10
23	Substrate Recognition and Motion Mode Analyses of PFV Integrase in Complex with Viral DNA via Coarse-Grained Models. PLoS ONE, 2013, 8, e54929.	2.5	9
24	The global motion affecting electron transfer in <i>Plasmodium falciparum</i> type II NADH dehydrogenases: a novel non-competitive mechanism for quinoline ketone derivative inhibitors. Physical Chemistry Chemical Physics, 2019, 21, 18105-18118.	2.8	9
25	Applications of Molecular Simulation in the Discovery of Antituberculosis Drugs: A Review. Protein and Peptide Letters, 2019, 26, 648-663.	0.9	9
26	BP[dG]-induced distortions to DNA polymerase and DNA duplex: A detailed mechanism of BP adducts blocking replication. Food and Chemical Toxicology, 2020, 140, 111325.	3.6	8
27	Theoretical insight into the photodeactivation pathway of the tetradentate Pt(II) complex: The l€â€€onjugation effect. Applied Organometallic Chemistry, 2018, 32, e4220.	3.5	7
28	Theoretical insight into the photodeactivation pathway of the tetradentate Pt (II) complex with different inductive substituents. Applied Organometallic Chemistry, 2019, 33, e4879.	3.5	7
29	Classification and Design of HIV-1 Integrase Inhibitors Based on Machine Learning. Computational and Mathematical Methods in Medicine, 2021, 2021, 1-11.	1.3	6
30	C- and N-Adducts of N-alkenyl substituted Arduengo carbene and N-alkyl substituted imidazole with PF5: synthesis and structural investigation. Russian Chemical Bulletin, 2014, 63, 2668-2674.	1.5	5
31	Inhibition Mechanism of Indoleamine 2, 3-Dioxygenase 1 (IDO1) by Amidoxime Derivatives and Its Revelation in Drug Design: Comparative Molecular Dynamics Simulations. Frontiers in Molecular Biosciences, 2019, 6, 164.	3.5	5
32	Research progress of human AP endonuclease 1: structure, catalytic mechanism and inhibitors. Current Protein and Peptide Science, 2022, 23, .	1.4	5
33	Design of stable platinum(II) complexes exhibited various colors via auxiliary ligand and electron-donating/withdrawing groups: A theoretical investigation. Organic Electronics, 2019, 71, 251-257.	2.6	4
34	Specifically targeting Mtb cell-wall and TMM transporter: the development of MmpL3 inhibitors. Current Protein and Peptide Science, 2021, 22, 290-303.	1.4	4
35	Allosteric and transport modulation of human concentrative nucleoside transporter 3 at the atomic scale. Physical Chemistry Chemical Physics, 2021, 23, 25401-25413.	2.8	4
36	An effective HIV-1 integrase inhibitor screening platform: Rationality validation of drug screening, conformational mobility and molecular recognition analysis for PFV integrase complex with viral DNA. Journal of Molecular Graphics and Modelling, 2017, 78, 96-109.	2.4	3

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37	Non-synonymous substitution of evolutionarily conserved residue in Tau class glutathione transferases alters structural and catalytic features. International Journal of Biological Macromolecules, 2022, 197, 39-48.	7.5	3
38	A potential strategy used for controlling the phosphorescence quantum yield of cyclometalated (CˆC*) platinum(II) NHC complexes: The theoretical insight. Organic Electronics, 2018, 57, 367-376.	2.6	2
39	Influence of restricted rotation of small-sized substituent on phosphorescence efficiency for Pt(II) complexes: A theoretical investigation. Organic Electronics, 2018, 61, 25-34.	2.6	2
40	Potential strategy used for controlling the phosphorescent properties in tetradentate Pt(II) complexes: Effect of azole ligand. Applied Organometallic Chemistry, 2019, 33, e5125.	3.5	2
41	An Overview of Computational Tools of Nucleic Acid Binding Site Prediction for Site-specific Proteins and Nucleases. Protein and Peptide Letters, 2020, 27, 370-384.	0.9	2
42	In vitro selection and identification of a cold-tolerant variant in pineapple (Ananas comosus). Horticulture Environment and Biotechnology, 2022, 63, 275.	2.1	2
43	A novel ligand swing-mediated active site coordination change of human apurinic/apyrimidinic endonuclease 1: A potential cytotoxic mechanism of nickel ion in the base excision repair. Chemical Physics, 2022, 555, 111456.	1.9	2
44	Molecular basis for substrate recognition by the bacterial nucleoside transporter NupG. Journal of Biological Chemistry, 2021, 296, 100479.	3.4	1
45	A promising strategy for increasing phosphorescent quantum yield: The ligand 10 yclic chelate of the tetradentate Pt(II) complex. Applied Organometallic Chemistry, 2022, 36, .	3.5	1
46	Immunotherapy: MAPKâ€Targeted Drug Delivered by a pHâ€Sensitive MSNP Nanocarrier Synergizes with PDâ€I Blockade in Melanoma without Tâ€Cell Suppression (Adv. Funct. Mater. 12/2019). Advanced Functional Materials, 2019, 29, 1970079.	14.9	0
47	Phosphine ligand-coated Cu nanoparticle-catalyzed selective semihydrogenation of alkynes: electronic or hindrance effects of the ligand?. Physical Chemistry Chemical Physics, 2020, 22, 16905-16913.	2.8	0
48	DFT insight into Hashmi phenol synthesis catalyzed by Au single-walled nanotubes: mechanism and charge effect. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	0