Chung F Wong

List of Publications by Year
in descending order

59 papers	1,553 citations	257450 24 h-index	330143 37 g-index
59 all docs	59 docs citations	59 times ranked	1592 citing authors

#	Article	IF	Citations
1	Qualitative Prediction of Ligand Dissociation Kinetics from Focal Adhesion Kinase Using Steered Molecular Dynamics. Life, 2021, 11, 74.	2.4	14
2	EDockâ€ML: A web server for using ensemble docking with machine learning to aid drug discovery. Protein Science, 2021, 30, 1087-1097.	7.6	5
3	Why heptakis(2,3-di-O-acetyl)-Î²-cyclodextrin can separate terbutaline enantiomers better than Î²-cyclodextrin: nonbonding and hydrophobic interactions. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2021, 100, 189.	1.6	5
4	Using machine learning to improve ensemble docking for drug discovery. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1263-1270.	2.6	18
5	Improving ensemble docking for drug discovery by machine learning. Journal of Theoretical and Computational Chemistry, 2019, 18, 1920001.	1.8	7
6	Steered molecular dynamics simulations for uncovering the molecular mechanisms of drug dissociation and for drug screening: A test on the focal adhesion kinase. Journal of Computational Chemistry, 2018, 39, 1307-1318.	3.3	22
7	Program for Simulating Gel Electrophoresis of Enzyme-Digested Proteins. Journal of Chemical Education, 2018, 95, 2064-2067.	2.3	1
8	Conformational transition paths harbor structures useful for aiding drug discovery and understanding enzymatic mechanisms in protein kinases. Protein Science, 2016, 25, 192-203.	7.6	5
9	Variable van der Waals Radii Derived From a Hybrid Gaussian Charge Distribution Model for Continuum-Solvent Electrostatic Calculations. Zeitschrift Fur Physikalische Chemie, 2016, 230, 681-701.	2.8	2
10	Inexpensive Method for Selecting Receptor Structures for Virtual Screening. Journal of Chemical Information and Modeling, 2016, 56, 21-34.	5.4	37
11	Flexible receptor docking for drug discovery. Expert Opinion on Drug Discovery, 2015, 10, 1189-1200.	5.0	62
12	Incorporating Receptor Flexibility into Structure-Based Drug Discovery. Methods in Pharmacology and Toxicology, 2015, , 65-84.	0.2	1
13	A new class of salicylic acid derivatives for inhibiting YopH of Yersinia pestis. Bioorganic and Medicinal Chemistry, 2014, 22, 6781-6788.	3.0	2
14	Molecular simulation of drug-binding kinetics. Molecular Simulation, 2014, 40, 889-903.	2.0	9
15	Drug Design for Protein Kinases and Phosphatases: Flexible-Receptor Docking, Binding Affinity and Specificity, and Drug-Binding Kinetics. Current Pharmaceutical Design, 2013, 19, 4739-4754.	1.9	20
16	Simulation reveals two major docking pathways between the hexapeptide GDYMNM and the catalytic domain of the insulin receptor protein kinase. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2275-2286.	2.6	5
17	A Case Study of Scoring and Rescoring in Peptide Docking. Methods in Molecular Biology, 2012, 819, 269-293.	0.9	3
18	Incorporating Protein Flexibility in Molecular Docking by Molecular Dynamics: Applications to Protein Kinase and Phosphatase Systems. , 2011, , 219-249.		1

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19	Influence of kinetics of drug binding on EGFR signaling: A comparative study of three EGFR signaling pathway models. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2491-2504.	2.6	17
20	Derivatives of Salicylic Acid as Inhibitors of YopH in Yersinia pestis. Chemical Biology and Drug Design, 2010, 76, 85-99.	3.2	24
21	SUPPLEMENTING THE PBSA APPROACH WITH QUANTUM MECHANICS TO STUDY THE BINDING BETWEEN CDK2 AND N²-SUBSTITUTED O⁶-CYCLOHEXYLMETHOXYGUANINE INHIBITORS. Journal of Theoretical and Computational Chemistry, 2010, 09, 543-559.	1.8	12
22	Conformational selection of protein kinase A revealed by flexibleâ€ligand flexibleâ€protein docking. Journal of Computational Chemistry, 2009, 30, 631-644.	3.3	22
23	Docking Flexible Peptide to Flexible Protein by Molecular Dynamics Using Two Implicit-Solvent Models: An Evaluation in Protein Kinase and Phosphatase Systems. Journal of Physical Chemistry B, 2009, 113, 14343-14354.	2.6	31
24	Beyond Thermodynamics: Drug Binding Kinetics Could Influence Epidermal Growth Factor Signaling. Journal of Medicinal Chemistry, 2009, 52, 5582-5585.	6.4	18
25	Release of ADP from the catalytic subunit of protein kinase A: A molecular dynamics simulation study. Protein Science, 2009, 14, 159-168.	7.6	33
26	A Computational Study of the Phosphorylation Mechanism of the Insulin Receptor Tyrosine Kinase. Journal of Physical Chemistry A, 2009, 113, 5144-5150.	2.5	14
27	Flexible proteinâ€“flexible ligand docking with disrupted velocity simulated annealing. Proteins: Structure, Function and Bioinformatics, 2008, 71, 440-454.	2.6	30
28	Flexible ligandâ€“flexible protein docking in protein kinase systems. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2008, 1784, 244-251.	2.3	39
29	Sensitivity Analysis in Biomolecular Simulation. Reviews in Computational Chemistry, 2007, , 281-326.	1.5	11
30	A Mining Minima Approach to Exploring the Docking Pathways of p-Nitrocatechol Sulfate to YopH. Biophysical Journal, 2007, 93, 4141-4150.	0.5	17
31	Relative contributions of desolvation, inter- and intramolecular interactions to binding affinity in protein kinase systems. Journal of Computational Chemistry, 2005, 26, 668-681.	3.3	28
32	Molecular docking of balanol to dynamics snapshots of protein kinase A. Proteins: Structure, Function and Bioinformatics, 2005, 61, 850-858.	2.6	60
33	Charge optimization of the interface between protein kinases and their ligands. Journal of Computational Chemistry, 2004, 25, 1416-1429.	3.3	36
34	Brownian dynamics simulations of ion atmospheres around polyalanine and B-DNA: Effects of biomolecular dielectric. Biopolymers, 2003, 70, 391-402.	2.4	11
35	PROTEINFLEXIBILITY ANDCOMPUTER-AIDEDDRUGDESIGN. Annual Review of Pharmacology and Toxicology, 2003, 43, 31-45.	9.4	71
36	Protein Simulation and Drug Design. Advances in Protein Chemistry, 2003, 66, 87-121.	4.4	36

#	Article	IF	Citations
37	A Computational Model of Binding Thermodynamics:Â The Design of Cyclin-dependent Kinase 2 Inhibitors. Journal of Medicinal Chemistry, 2003, 46, 3314-3325.	6.4	37
38	COMPUTATIONAL ANALYSIS OF THE INTERACTIONS BETWEEN THE ANGIOGENESIS INHIBITOR PD173074 AND FIBROBLAST GROWTH FACTOR RECEPTOR 1. Journal of Theoretical and Computational Chemistry, 2003, 02, 43-56.	1.8	1
39	Entropy Loss of Hydroxyl Groups of Balanol upon Binding to Protein Kinase A. Journal of Chemical Education, 2002, 79, 1122.	2.3	5
40	Designing specific protein kinase inhibitors:. , 2002, 93, 169-178.		23
41	Atomistic Brownian Dynamics Simulation of Peptide Phosphorylation. Journal of the American Chemical Society, 2001, 123, 9107-9111.	13.7	50
42	Computational Analysis of PKAâ^'Balanol Interactions. Journal of Medicinal Chemistry, 2001, 44, 1530-1539.	6.4	33
43	The structure of Sky1p reveals a novel mechanism for constitutive activity. Nature Structural Biology, 2001, 8, 176-183.	9.7	70
44	Classical and Quantum Simulations of Tryptophan in Solution. Journal of Physical Chemistry A, 1997, 101, 1935-1945.	2.5	29
45	Predicting helical segments in proteins by a helix-coil transition theory with parameters derived from a structural database of proteins. Proteins: Structure, Function and Bioinformatics, 1997, 28, 344-359.	2.6	12
46	Brownian Dynamics Simulations of Polyalanine in Salt Solutions. The Journal of Physical Chemistry, 1996, 100, 15280-15289.	2.9	10
47	Parametric sensitivity analysis of avian pancreatic polypeptide (APP). Proteins: Structure, Function and Bioinformatics, 1995, 23, 218-232.	2.6	16
48	Sensitivity Analysis of a Two-Dimensional Square Lattice Model of Protein Folding. The Journal of Physical Chemistry, 1995, 99, 3379-3386.	2.9	9
49	Sensitivity Analysis of a Polarizable Water Model. The Journal of Physical Chemistry, 1994, 98, 4695-4701.	2.9	25
50	Cytochrome c: a molecular proving ground for computer simulations. The Journal of Physical Chemistry, 1993, 97, 3100-3110.	2.9	30
51	Sensitivity analysis of distribution functions of liquid water. Journal of Chemical Physics, 1993, 99, 9047-9053.	3.0	20
52	Sensitivity analysis of water thermodynamics. Journal of Chemical Physics, 1993, 98, 8892-8899.	3.0	47
53	Fluctuation of the solvent-accessible surface area of tuna ferrocytochrome c. Biopolymers, 1990, 29, 1877-1883.	2.4	10
54	Partial electrostatic charges for the active center of Cu, Zn superoxide dismutase. Journal of Computational Chemistry, 1990, 11, 346-350.	3.3	31

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55	Hydration of superoxide studied by molecular dynamics simulation. Journal of Computational Chemistry, 1990, 11, 1003-1008.	3.3	9
56	Superoxide dismutase: Fluctuations in the structure and solvation of the active site channel studied by molecular dynamics simulation. Biopolymers, 1989, 28, 2085-2096.	2.4	28
57	Quantum simulation of ferrocytochrome c. Nature, 1988, 334, 726-728.	27.8	18
58	Dynamics and design of enzymes and inhibitors. Journal of the American Chemical Society, 1986, 108, 3830-3832.	13.7	259
59	Computer Simulation and the Design of New Biological Molecules. Israel Journal of Chemistry, 1986, 27, 211-215.	2.3	52