

# Chung F Wong

## List of Publications by Year in descending order

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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	Dynamics and design of enzymes and inhibitors. <i>Journal of the American Chemical Society</i> , 1986, 108, 3830-3832.	13.7	259
2	PROTEINFLEXIBILITY ANDCOMPUTER-AIDEDDRUGDESIGN. <i>Annual Review of Pharmacology and Toxicology</i> , 2003, 43, 31-45.	9.4	71
3	The structure of Sky1p reveals a novel mechanism for constitutive activity. <i>Nature Structural Biology</i> , 2001, 8, 176-183.	9.7	70
4	Flexible receptor docking for drug discovery. <i>Expert Opinion on Drug Discovery</i> , 2015, 10, 1189-1200.	5.0	62
5	Molecular docking of balanol to dynamics snapshots of protein kinase A. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 61, 850-858.	2.6	60
6	Computer Simulation and the Design of New Biological Molecules. <i>Israel Journal of Chemistry</i> , 1986, 27, 211-215.	2.3	52
7	Atomistic Brownian Dynamics Simulation of Peptide Phosphorylation. <i>Journal of the American Chemical Society</i> , 2001, 123, 9107-9111.	13.7	50
8	Sensitivity analysis of water thermodynamics. <i>Journal of Chemical Physics</i> , 1993, 98, 8892-8899.	3.0	47
9	Flexible ligand flexible protein docking in protein kinase systems. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2008, 1784, 244-251.	2.3	39
10	A Computational Model of Binding Thermodynamics: The Design of Cyclin-dependent Kinase 2 Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2003, 46, 3314-3325.	6.4	37
11	Inexpensive Method for Selecting Receptor Structures for Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 21-34.	5.4	37
12	Protein Simulation and Drug Design. <i>Advances in Protein Chemistry</i> , 2003, 66, 87-121.	4.4	36
13	Charge optimization of the interface between protein kinases and their ligands. <i>Journal of Computational Chemistry</i> , 2004, 25, 1416-1429.	3.3	36
14	Computational Analysis of PKA Balanol Interactions. <i>Journal of Medicinal Chemistry</i> , 2001, 44, 1530-1539.	6.4	33
15	Release of ADP from the catalytic subunit of protein kinase A: A molecular dynamics simulation study. <i>Protein Science</i> , 2009, 14, 159-168.	7.6	33
16	Partial electrostatic charges for the active center of Cu, Zn superoxide dismutase. <i>Journal of Computational Chemistry</i> , 1990, 11, 346-350.	3.3	31
17	Docking Flexible Peptide to Flexible Protein by Molecular Dynamics Using Two Implicit-Solvent Models: An Evaluation in Protein Kinase and Phosphatase Systems. <i>Journal of Physical Chemistry B</i> , 2009, 113, 14343-14354.	2.6	31
18	Cytochrome c: a molecular proving ground for computer simulations. <i>The Journal of Physical Chemistry</i> , 1993, 97, 3100-3110.	2.9	30

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19	Flexible proteinâ€“flexible ligand docking with disrupted velocity simulated annealing. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 440-454.	2.6	30
20	Classical and Quantum Simulations of Tryptophan in Solution. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1935-1945.	2.5	29
21	Superoxide dismutase: Fluctuations in the structure and solvation of the active site channel studied by molecular dynamics simulation. <i>Biopolymers</i> , 1989, 28, 2085-2096.	2.4	28
22	Relative contributions of desolvation, inter- and intramolecular interactions to binding affinity in protein kinase systems. <i>Journal of Computational Chemistry</i> , 2005, 26, 668-681.	3.3	28
23	Sensitivity Analysis of a Polarizable Water Model. <i>The Journal of Physical Chemistry</i> , 1994, 98, 4695-4701.	2.9	25
24	Derivatives of Salicylic Acid as Inhibitors of YopH in <i>Yersinia pestis</i> . <i>Chemical Biology and Drug Design</i> , 2010, 76, 85-99.	3.2	24
25	Designing specific protein kinase inhibitors. , 2002, 93, 169-178.		23
26	Conformational selection of protein kinase A revealed by flexibleâ€“ligand flexibleâ€“protein docking. <i>Journal of Computational Chemistry</i> , 2009, 30, 631-644.	3.3	22
27	Steered molecular dynamics simulations for uncovering the molecular mechanisms of drug dissociation and for drug screening: A test on the focal adhesion kinase. <i>Journal of Computational Chemistry</i> , 2018, 39, 1307-1318.	3.3	22
28	Sensitivity analysis of distribution functions of liquid water. <i>Journal of Chemical Physics</i> , 1993, 99, 9047-9053.	3.0	20
29	Drug Design for Protein Kinases and Phosphatases: Flexible-Receptor Docking, Binding Affinity and Specificity, and Drug-Binding Kinetics. <i>Current Pharmaceutical Design</i> , 2013, 19, 4739-4754.	1.9	20
30	Quantum simulation of ferrocycytochrome c. <i>Nature</i> , 1988, 334, 726-728.	27.8	18
31	Beyond Thermodynamics: Drug Binding Kinetics Could Influence Epidermal Growth Factor Signaling. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 5582-5585.	6.4	18
32	Using machine learning to improve ensemble docking for drug discovery. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 1263-1270.	2.6	18
33	A Mining Minima Approach to Exploring the Docking Pathways of p-Nitrocatechol Sulfate to YopH. <i>Biophysical Journal</i> , 2007, 93, 4141-4150.	0.5	17
34	Influence of kinetics of drug binding on EGFR signaling: A comparative study of three EGFR signaling pathway models. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 2491-2504.	2.6	17
35	Parametric sensitivity analysis of avian pancreatic polypeptide (APP). <i>Proteins: Structure, Function and Bioinformatics</i> , 1995, 23, 218-232.	2.6	16
36	A Computational Study of the Phosphorylation Mechanism of the Insulin Receptor Tyrosine Kinase. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5144-5150.	2.5	14

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37	Qualitative Prediction of Ligand Dissociation Kinetics from Focal Adhesion Kinase Using Steered Molecular Dynamics. <i>Life</i> , 2021, 11, 74.	2.4	14
38	Predicting helical segments in proteins by a helix-coil transition theory with parameters derived from a structural database of proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 1997, 28, 344-359.	2.6	12
39	SUPPLEMENTING THE PBSA APPROACH WITH QUANTUM MECHANICS TO STUDY THE BINDING BETWEEN CDK2 AND $N^{2}$ -SUBSTITUTED $O^{6}$ -CYCLOHEXYLMETHOXYGUANINE INHIBITORS. <i>Journal of Theoretical and Computational Chemistry</i> , 2010, 09, 543-559.	1.8	12
40	Brownian dynamics simulations of ion atmospheres around polyaniline and B-DNA: Effects of biomolecular dielectric. <i>Biopolymers</i> , 2003, 70, 391-402.	2.4	11
41	Sensitivity Analysis in Biomolecular Simulation. <i>Reviews in Computational Chemistry</i> , 2007, , 281-326.	1.5	11
42	Fluctuation of the solvent-accessible surface area of tuna ferrocytochrome c. <i>Biopolymers</i> , 1990, 29, 1877-1883.	2.4	10
43	Brownian Dynamics Simulations of Polyaniline in Salt Solutions. <i>The Journal of Physical Chemistry</i> , 1996, 100, 15280-15289.	2.9	10
44	Hydration of superoxide studied by molecular dynamics simulation. <i>Journal of Computational Chemistry</i> , 1990, 11, 1003-1008.	3.3	9
45	Sensitivity Analysis of a Two-Dimensional Square Lattice Model of Protein Folding. <i>The Journal of Physical Chemistry</i> , 1995, 99, 3379-3386.	2.9	9
46	Molecular simulation of drug-binding kinetics. <i>Molecular Simulation</i> , 2014, 40, 889-903.	2.0	9
47	Improving ensemble docking for drug discovery by machine learning. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1920001.	1.8	7
48	Entropy Loss of Hydroxyl Groups of Balanol upon Binding to Protein Kinase A. <i>Journal of Chemical Education</i> , 2002, 79, 1122.	2.3	5
49	Simulation reveals two major docking pathways between the hexapeptide GDYMMN and the catalytic domain of the insulin receptor protein kinase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 2275-2286.	2.6	5
50	Conformational transition paths harbor structures useful for aiding drug discovery and understanding enzymatic mechanisms in protein kinases. <i>Protein Science</i> , 2016, 25, 192-203.	7.6	5
51	EDock $\hat{e}$ ML: A web server for using ensemble docking with machine learning to aid drug discovery. <i>Protein Science</i> , 2021, 30, 1087-1097.	7.6	5
52	Why heptakis(2,3-di-O-acetyl)- $\hat{I}^2$ -cyclodextrin can separate terbutaline enantiomers better than $\hat{I}^2$ -cyclodextrin: nonbonding and hydrophobic interactions. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2021, 100, 189.	1.6	5
53	A Case Study of Scoring and Rescoring in Peptide Docking. <i>Methods in Molecular Biology</i> , 2012, 819, 269-293.	0.9	3
54	A new class of salicylic acid derivatives for inhibiting YopH of <i>Yersinia pestis</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2014, 22, 6781-6788.	3.0	2

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55	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
56	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
57	Incorporating Protein Flexibility in Molecular Docking by Molecular Dynamics: Applications to Protein Kinase and Phosphatase Systems. , 2011, , 219-249.		1
58	Incorporating Receptor Flexibility into Structure-Based Drug Discovery. Methods in Pharmacology and Toxicology, 2015, , 65-84.	0.2	1
59	Program for Simulating Gel Electrophoresis of Enzyme-Digested Proteins. Journal of Chemical Education, 2018, 95, 2064-2067.	2.3	1