Piotr Cieplak

List of Publications by Year in Descending Order

69 papers	25,741 citations	29 h-index	71 g-index
71 ext. papers	27,997 ext. citations	5.3 avg, IF	6.17 L-index

#	Paper	IF	Citations
69	S-Nitrosylation of p62 Inhibits Autophagic Flux to Promote α-Synuclein Secretion and Spread in Parkinson's Disease and Lewy Body Dementia.. *Journal of Neuroscience*, **2022**,	6.6	3
68	Stress tensor and constant pressure simulation for polarizable Gaussian multipole model.. *Journal of Chemical Physics*, **2022**, 156, 114114	3.9	0
67	S-nitrosylated TDP-43 triggers aggregation, cell-to-cell spread, and neurotoxicity in hiPSCs and in vivo models of ALS/FTD. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	10
66	Toxoplasma gondii serine hydrolases regulate parasite lipid mobilization during growth and replication within the host. *Cell Chemical Biology*, **2021**, 28, 1501-1513.e5	8.2	0
65	Epitope-resolved profiling of the SARS-CoV-2 antibody response identifies cross-reactivity with endemic human coronaviruses. *Cell Reports Medicine*, **2021**, 2, 100189	18	80
64	Quantitative profiling of protease specificity. *PLoS Computational Biology*, **2021**, 17, e1008101	5	2
63	Determining the atomic charge of calcium ion requires the information of its coordination geometry in an EF-hand motif. *Journal of Chemical Physics*, **2021**, 154, 124104	3.9	5
62	The Antimalarial Natural Product Salinipostin A Identifies Essential α/β Serine Hydrolases Involved in Lipid Metabolism in P. falciparum Parasites. *Cell Chemical Biology*, **2020**, 27, 143-157.e5	8.2	27
61	A Note on the Potential BCG Vaccination – COVID-19 Molecular Link. *Coronaviruses*, **2020**, 1, 4-6	1.5	2
60	Epitope-resolved profiling of the SARS-CoV-2 antibody response identifies cross-reactivity with an endemic human CoV **2020**,		14
59	Efficient formulation of polarizable Gaussian multipole electrostatics for biomolecular simulations. *Journal of Chemical Physics*, **2020**, 153, 114116	3.9	9
58	Interactions between motor domains in kinesin-14 Ncd - a molecular dynamics study. *Biochemical Journal*, **2019**, 476, 2449-2462	3.8	
57	Development of Polarizable Gaussian Model for Molecular Mechanical Calculations I: Atomic Polarizability Parameterization To Reproduce ab Initio Anisotropy. *Journal of Chemical Theory and Computation*, **2019**, 15, 1146-1158	6.4	15
56	Effect of phosphorylation and single nucleotide polymorphisms on caspase substrates processing. *Apoptosis: an International Journal on Programmed Cell Death*, **2018**, 23, 194-200	5.4	7
55	Amino acid sequence conservation of the algesic fragment of myelin basic protein is required for its interaction with CDK5 and function in pain. *FEBS Journal*, **2018**, 285, 3485-3502	5.7	4
54	Role of N-glycosylation in activation of proMMP-9. A molecular dynamics simulations study. *PLoS ONE*, **2018**, 13, e0191157	3.7	7
53	Interaction of the cryptic fragment of myelin basic protein with mitochondrial voltage-dependent anion-selective channel-1 affects cell energy metabolism. *Biochemical Journal*, **2018**, 475, 2355-2376	3.8	3

52	Matrix metalloproteinases - From the cleavage data to the prediction tools and beyond. *Biochimica Et Biophysica Acta - Molecular Cell Research*, **2017**, 1864, 1952-1963	4.9	24
51	Resolving the Ligand-Binding Specificity in c-MYC G-Quadruplex DNA: Absolute Binding Free Energy Calculations and SPR Experiment. *Journal of Physical Chemistry B*, **2017**, 121, 10484-10497	3.4	28
50	Induced polarization restricts the conformational distribution of a light-harvesting molecular triad in the ground state. *Physical Chemistry Chemical Physics*, **2017**, 19, 22969-22980	3.6	10
49	Selective function-blocking monoclonal human antibody highlights the important role of membrane type-1 matrix metalloproteinase (MT1-MMP) in metastasis. *Oncotarget*, **2017**, 8, 2781-2799	3.3	29
48	CaspNeuroD: a knowledgebase of predicted caspase cleavage sites in human proteins related to neurodegenerative diseases. *Database: the Journal of Biological Databases and Curation*, **2016**, 2016,	5	4
47	Letter to the Editor: Caspase cleavage sites in the human proteome: CaspDB, a database of predicted substrates. *Apoptosis: an International Journal on Programmed Cell Death*, **2015**, 20, 421	5.4	3
46	High-Throughput Multiplexed Peptide-Centric Profiling Illustrates Both Substrate Cleavage Redundancy and Specificity in the MMP Family. *Chemistry and Biology*, **2015**, 22, 1122-33		21
45	Matrix Metalloproteinase (MMP) Proteolysis of the Extracellular Loop of Voltage-gated Sodium Channels and Potential Alterations in Pain Signaling. *Journal of Biological Chemistry*, **2015**, 290, 22939-44	5.4	8
44	CleavPredict: A Platform for Reasoning about Matrix Metalloproteinases Proteolytic Events. *PLoS ONE*, **2015**, 10, e0127877	3.7	27
43	Basis for substrate recognition and distinction by matrix metalloproteinases. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, E4148-55	11.5	49
42	S-nitrosylation-mediated redox transcriptional switch modulates neurogenesis and neuronal cell death. *Cell Reports*, **2014**, 8, 217-28	10.6	48
41	Sequence-derived structural features driving proteolytic processing. *Proteomics*, **2014**, 14, 42-50	4.8	14
40	Caspase cleavage sites in the human proteome: CaspDB, a database of predicted substrates. *PLoS ONE*, **2014**, 9, e110539	3.7	47
39	Peptide Sequence Region That is Essential for the Interactions of the Enterotoxigenic Bacteroides fragilis Metalloproteinase II with E-cadherin **2014**, 1, 3-14		2
38	Development of polarizable models for molecular mechanical calculations. 3. Polarizable water models conforming to Thole polarization screening schemes. *Journal of Physical Chemistry B*, **2012**, 116, 7999-8008	3.4	42
37	Development of polarizable models for molecular mechanical calculations. 4. van der Waals parametrization. *Journal of Physical Chemistry B*, **2012**, 116, 7088-101	3.4	44
36	Development of polarizable models for molecular mechanical calculations I: parameterization of atomic polarizability. *Journal of Physical Chemistry B*, **2011**, 115, 3091-9	3.4	114
35	Development of polarizable models for molecular mechanical calculations II: induced dipole models significantly improve accuracy of intermolecular interaction energies. *Journal of Physical Chemistry B*, **2011**, 115, 3100-11	3.4	101

34	Structural determinants of limited proteolysis. *Journal of Proteome Research*, **2011**, 10, 3642-51	5.6	44
33	The Wnt/planar cell polarity protein-tyrosine kinase-7 (PTK7) is a highly efficient proteolytic target of membrane type-1 matrix metalloproteinase: implications in cancer and embryogenesis. *Journal of Biological Chemistry*, **2010**, 285, 35740-9	5.4	65
32	Identifying protease cleavage sites by label-free mass spectrometry. *FASEB Journal*, **2010**, 24, 905.4	0.9	
31	Matrix metalloproteinase proteolysis of the myelin basic protein isoforms is a source of immunogenic peptides in autoimmune multiple sclerosis. *PLoS ONE*, **2009**, 4, e4952	3.7	67
30	Novel procedure for thermal equilibration in molecular dynamics simulation. *Molecular Simulation*, **2009**, 35, 349-357	2	9
29	Inflammatory proprotein convertase-matrix metalloproteinase proteolytic pathway in antigen-presenting cells as a step to autoimmune multiple sclerosis. *Journal of Biological Chemistry*, **2009**, 284, 30615-26	5.4	35
28	Polarization effects in molecular mechanical force fields. *Journal of Physics Condensed Matter*, **2009**, 21, 333102	1.8	192
27	High throughput substrate phage display for protease profiling. *Methods in Molecular Biology*, **2009** , 539, 93-114	1.4	22
26	Strike a balance: optimization of backbone torsion parameters of AMBER polarizable force field for simulations of proteins and peptides. *Journal of Computational Chemistry*, **2006**, 27, 781-90	3.5	138
25	Penultimate unit effects in the free-radical copolymerization of styrene with acrylonitrile according to theoretical thermochemistry. *Journal of Polymer Science Part A*, **2002**, 40, 3592-3603	2.5	15
24	Application of the Free Energy Calculations to Study Drug-enzyme and Drug-dna Complexes. *Molecular Simulation*, **2002**, 28, 173-186	2	2
23	AmberFFC, a flexible program to convert AMBER and GLYCAM force fields for use with commercial molecular modeling packages. *Journal of Molecular Modeling*, **2001**, 7, 422-432	2	9
22	Molecular mechanical models for organic and biological systems going beyond the atom centered two body additive approximation: aqueous solution free energies of methanol and N-methyl acetamide, nucleic acid base, and amide hydrogen bonding and chloroform/water partition coefficients of the nucleic acid bases. *Journal of Computational Chemistry*, **2001**, 22, 1048-1057	3.5	338
21	Calculating structures and free energies of complex molecules: combining molecular mechanics and continuum models. *Accounts of Chemical Research*, **2000**, 33, 889-97	24.3	3346
20	A modified version of the Cornell et al. force field with improved sugar pucker phases and helical repeat. *Journal of Biomolecular Structure and Dynamics*, **1999**, 16, 845-62	3.6	810
19	Continuum Solvent Studies of the Stability of DNA, RNA, and Phosphoramidate□DNA Helices. *Journal of the American Chemical Society*, **1998**, 120, 9401-9409	16.4	1269
18	Molecular Dynamics Simulations Find That 3□Phosphoramidate Modified DNA Duplexes Undergo a B to A Transition and Normal DNA Duplexes an A to B Transition. *Journal of the American Chemical Society*, **1997**, 119, 6722-6730	16.4	73
17	Molecular Design of Fluorine-Containing Peptide Mimetics. *ACS Symposium Series*, **1996**, 143-156	0.4	6

16	Elucidating the Origin of Conformational Energy Differences in Substituted 1,3-Dioxanes: A Combined Theoretical and Experimental Study. *Journal of Organic Chemistry*, **1996**, 61, 3662-3668	4.2	15
15	A technique to study molecular recognition in drug design: preliminary application of free energy derivatives to inhibition of a malarial cysteine protease. *Journal of Molecular Recognition*, **1996**, 9, 103-12	2.6	4
14	A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. *Journal of the American Chemical Society*, **1995**, 117, 5179-5197	16.4	10990
13	A molecular mechanical model that reproduces the relative energies for chair and twist-boat conformations of 1,3-dioxanes. *Journal of Computational Chemistry*, **1995**, 16, 243-261	3.5	33
12	Application of the multimolecule and multiconformational RESP methodology to biopolymers: Charge derivation for DNA, RNA, and proteins. *Journal of Computational Chemistry*, **1995**, 16, 1357-1377	3.5	820
11	Walking on the free energy hypersurface of the 18-crown-6 ion system using free energy derivatives. *Journal of Chemical Physics*, **1994**, 101, 627-633	3.9	16
10	Application of RESP charges to calculate conformational energies, hydrogen bond energies, and free energies of solvation. *Journal of the American Chemical Society*, **1993**, 115, 9620-9631	16.4	1031
9	A well-behaved electrostatic potential based method using charge restraints for deriving atomic charges: the RESP model. *The Journal of Physical Chemistry*, **1993**, 97, 10269-10280		5269
8	Hydration of Benzoic Acid in Benzene Solution. *Zeitschrift Fur Physikalische Chemie*, **1992**, 177, 63-74	3.1	2
7	On the use of electrostatic potential derived charges in molecular mechanics force fields. The relative solvation free energy of cis- and trans-N-methyl-acetamide. *Journal of Computational Chemistry*, **1991**, 12, 1232-1236	3.5	96
6	Free energy calculation on base specificity of drug--DNA interactions: application to daunomycin and acridine intercalation into DNA. *Biopolymers*, **1990**, 29, 717-27	2.2	49
5	Monte Carlo simulation of aqueous solutions of Li+ and Na+ using many-body potentials. Coordination numbers, ion solvation enthalpies, and the relative free energy of solvation. *Journal of Chemical Physics*, **1990**, 92, 6761-6767	3.9	63
4	Reply to: Comment on Water water and water ion potential functions including terms for many-body effects, T. P. Lybrand and P. Kollman, J. Chem. Phys. 83, 2923 (1985) and on Calculation of free energy changes in ion water clusters using nonadditive potential and the Monte Carlo methods, P. Cieplak, T. P. Lybrand, and P. Kollman, J. Chem. Phys. 86, 6393 (1987) *Journal of Chemical Physics*, **1988**, 88, 8017-8017	3.9	10
3	Conformations of duplex structures formed by oligodeoxynucleotides covalently linked to the intercalator 2-methoxy-6-chloro-9-aminoacridine. *Journal of Biomolecular Structure and Dynamics*, **1987**, 5, 361-82	3.6	11
2	Calculation of free energy changes in ion water clusters using nonadditive potentials and the Monte Carlo method. *Journal of Chemical Physics*, **1987**, 86, 6393-6403	3.9	77
1	Application of the quantum mechanics and free energy perturbation methods to study molecular processes. *International Journal of Quantum Chemistry*, **1987**, 32, 65-74	2.1	11