

# Piotr Cieplak

## List of Publications by Citations

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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	A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. <i>Journal of the American Chemical Society</i> , <b>1995</b> , 117, 5179-5197	16.4	10990
68	A well-behaved electrostatic potential based method using charge restraints for deriving atomic charges: the RESP model. <i>The Journal of Physical Chemistry</i> , <b>1993</b> , 97, 10269-10280		5269
67	Calculating structures and free energies of complex molecules: combining molecular mechanics and continuum models. <i>Accounts of Chemical Research</i> , <b>2000</b> , 33, 889-97	24.3	3346
66	Continuum Solvent Studies of the Stability of DNA, RNA, and Phosphoramidate DNA Helices. <i>Journal of the American Chemical Society</i> , <b>1998</b> , 120, 9401-9409	16.4	1269
65	Application of RESP charges to calculate conformational energies, hydrogen bond energies, and free energies of solvation. <i>Journal of the American Chemical Society</i> , <b>1993</b> , 115, 9620-9631	16.4	1031
64	Application of the multimolecule and multiconformational RESP methodology to biopolymers: Charge derivation for DNA, RNA, and proteins. <i>Journal of Computational Chemistry</i> , <b>1995</b> , 16, 1357-1377	3.5	820
63	A modified version of the Cornell et al. force field with improved sugar pucker phases and helical repeat. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>1999</b> , 16, 845-62	3.6	810
62	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. <i>Journal of Computational Chemistry</i> , <b>2001</b> , 22, 1048-1057	3.5	338
61	Polarization effects in molecular mechanical force fields. <i>Journal of Physics Condensed Matter</i> , <b>2009</b> , 21, 333102	1.8	192
60	Strike a balance: optimization of backbone torsion parameters of AMBER polarizable force field for simulations of proteins and peptides. <i>Journal of Computational Chemistry</i> , <b>2006</b> , 27, 781-90	3.5	138
59	Development of polarizable models for molecular mechanical calculations I: parameterization of atomic polarizability. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 3091-9	3.4	114
58	Development of polarizable models for molecular mechanical calculations II: induced dipole models significantly improve accuracy of intermolecular interaction energies. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 3100-11	3.4	101
57	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. <i>Journal of Computational Chemistry</i> , <b>1991</b> , 12, 1232-1236	3.5	96
56	Epitope-resolved profiling of the SARS-CoV-2 antibody response identifies cross-reactivity with endemic human coronaviruses. <i>Cell Reports Medicine</i> , <b>2021</b> , 2, 100189	18	80
55	Calculation of free energy changes in ion-water clusters using nonadditive potentials and the Monte Carlo method. <i>Journal of Chemical Physics</i> , <b>1987</b> , 86, 6393-6403	3.9	77
54	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. <i>Journal of the American Chemical Society</i> , <b>1997</b> , 119, 6722-6730	16.4	73
53	Matrix metalloproteinase proteolysis of the myelin basic protein isoforms is a source of immunogenic peptides in autoimmune multiple sclerosis. <i>PLoS ONE</i> , <b>2009</b> , 4, e4952	3.7	67

52	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. <i>Journal of Biological Chemistry</i> , <b>2010</b> , 285, 35740-9	5.4	65
51	Monte Carlo simulation of aqueous solutions of Li <sup>+</sup> and Na <sup>+</sup> using many-body potentials. Coordination numbers, ion solvation enthalpies, and the relative free energy of solvation. <i>Journal of Chemical Physics</i> , <b>1990</b> , 92, 6761-6767	3.9	63
50	Basis for substrate recognition and distinction by matrix metalloproteinases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2014</b> , 111, E4148-55	11.5	49
49	Free energy calculation on base specificity of drug-DNA interactions: application to daunomycin and acridine intercalation into DNA. <i>Biopolymers</i> , <b>1990</b> , 29, 717-27	2.2	49
48	S-nitrosylation-mediated redox transcriptional switch modulates neurogenesis and neuronal cell death. <i>Cell Reports</i> , <b>2014</b> , 8, 217-28	10.6	48
47	Caspase cleavage sites in the human proteome: CaspDB, a database of predicted substrates. <i>PLoS ONE</i> , <b>2014</b> , 9, e110539	3.7	47
46	Development of polarizable models for molecular mechanical calculations. 4. van der Waals parametrization. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 7088-101	3.4	44
45	Structural determinants of limited proteolysis. <i>Journal of Proteome Research</i> , <b>2011</b> , 10, 3642-51	5.6	44
44	Development of polarizable models for molecular mechanical calculations. 3. Polarizable water models conforming to Thole polarization screening schemes. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 7999-8008	3.4	42
43	Inflammatory proprotein convertase-matrix metalloproteinase proteolytic pathway in antigen-presenting cells as a step to autoimmune multiple sclerosis. <i>Journal of Biological Chemistry</i> , <b>2009</b> , 284, 30615-26	5.4	35
42	A molecular mechanical model that reproduces the relative energies for chair and twist-boat conformations of 1,3-dioxanes. <i>Journal of Computational Chemistry</i> , <b>1995</b> , 16, 243-261	3.5	33
41	Selective function-blocking monoclonal human antibody highlights the important role of membrane type-1 matrix metalloproteinase (MT1-MMP) in metastasis. <i>Oncotarget</i> , <b>2017</b> , 8, 2781-2799	3.3	29
40	Resolving the Ligand-Binding Specificity in c-MYC G-Quadruplex DNA: Absolute Binding Free Energy Calculations and SPR Experiment. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 10484-10497	3.4	28
39	The Antimalarial Natural Product Salinipostin A Identifies Essential Serine Hydrolases Involved in Lipid Metabolism in <i>P. falciparum</i> Parasites. <i>Cell Chemical Biology</i> , <b>2020</b> , 27, 143-157.e5	8.2	27
38	CleavPredict: A Platform for Reasoning about Matrix Metalloproteinases Proteolytic Events. <i>PLoS ONE</i> , <b>2015</b> , 10, e0127877	3.7	27
37	Matrix metalloproteinases - From the cleavage data to the prediction tools and beyond. <i>Biochimica Et Biophysica Acta - Molecular Cell Research</i> , <b>2017</b> , 1864, 1952-1963	4.9	24
36	High throughput substrate phage display for protease profiling. <i>Methods in Molecular Biology</i> , <b>2009</b> , 539, 93-114	1.4	22
35	High-Throughput Multiplexed Peptide-Centric Profiling Illustrates Both Substrate Cleavage Redundancy and Specificity in the MMP Family. <i>Chemistry and Biology</i> , <b>2015</b> , 22, 1122-33		21

34	Walking on the free energy hypersurface of the 18-crown-6 ion system using free energy derivatives. <i>Journal of Chemical Physics</i> , <b>1994</b> , 101, 627-633	3.9	16
33	Penultimate unit effects in the free-radical copolymerization of styrene with acrylonitrile according to theoretical thermochemistry. <i>Journal of Polymer Science Part A</i> , <b>2002</b> , 40, 3592-3603	2.5	15
32	Elucidating the Origin of Conformational Energy Differences in Substituted 1,3-Dioxanes: A Combined Theoretical and Experimental Study. <i>Journal of Organic Chemistry</i> , <b>1996</b> , 61, 3662-3668	4.2	15
31	Development of Polarizable Gaussian Model for Molecular Mechanical Calculations I: Atomic Polarizability Parameterization To Reproduce ab Initio Anisotropy. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 1146-1158	6.4	15
30	Sequence-derived structural features driving proteolytic processing. <i>Proteomics</i> , <b>2014</b> , 14, 42-50	4.8	14
29	Epitope-resolved profiling of the SARS-CoV-2 antibody response identifies cross-reactivity with an endemic human CoV <b>2020</b> ,		14
28	Conformations of duplex structures formed by oligodeoxynucleotides covalently linked to the intercalator 2-methoxy-6-chloro-9-aminoacridine. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>1987</b> , 5, 361-82	3.6	11
27	Application of the quantum mechanics and free energy perturbation methods to study molecular processes. <i>International Journal of Quantum Chemistry</i> , <b>1987</b> , 32, 65-74	2.1	11
26	Induced polarization restricts the conformational distribution of a light-harvesting molecular triad in the ground state. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 22969-22980	3.6	10
25	Reply to: Comment on Water-water and water-ion potential functions including terms for many-body effects, P. Lybrand and P. Kollman, <i>J. Chem. Phys.</i> 83, 2923 (1985) and on Calculation of free energy changes in ion-water clusters using nonadditive potential and the Monte Carlo method, P. Simola, P. Lybrand and P. Kollman, <i>J. Chem. Phys.</i> 86, 6203 (1987) <b>1987</b> , 6	3.9	10
24	S-nitrosylated TDP-43 triggers aggregation, cell-to-cell spread, and neurotoxicity in hiPSCs and in vivo models of ALS/FTD. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2021</b> , 118,	11.5	10
23	Novel procedure for thermal equilibration in molecular dynamics simulation. <i>Molecular Simulation</i> , <b>2009</b> , 35, 349-357	2	9
22	AmberFFC, a flexible program to convert AMBER and GLYCAM force fields for use with commercial molecular modeling packages. <i>Journal of Molecular Modeling</i> , <b>2001</b> , 7, 422-432	2	9
21	Efficient formulation of polarizable Gaussian multipole electrostatics for biomolecular simulations. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 114116	3.9	9
20	Matrix Metalloproteinase (MMP) Proteolysis of the Extracellular Loop of Voltage-gated Sodium Channels and Potential Alterations in Pain Signaling. <i>Journal of Biological Chemistry</i> , <b>2015</b> , 290, 22939-44	5.4	8
19	Effect of phosphorylation and single nucleotide polymorphisms on caspase substrates processing. <i>Apoptosis: an International Journal on Programmed Cell Death</i> , <b>2018</b> , 23, 194-200	5.4	7
18	Role of N-glycosylation in activation of proMMP-9. A molecular dynamics simulations study. <i>PLoS ONE</i> , <b>2018</b> , 13, e0191157	3.7	7
17	Molecular Design of Fluorine-Containing Peptide Mimetics. <i>ACS Symposium Series</i> , <b>1996</b> , 143-156	0.4	6

16	Determining the atomic charge of calcium ion requires the information of its coordination geometry in an EF-hand motif. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 124104	3.9	5
15	Amino acid sequence conservation of the algescic fragment of myelin basic protein is required for its interaction with CDK5 and function in pain. <i>FEBS Journal</i> , <b>2018</b> , 285, 3485-3502	5.7	4
14	A technique to study molecular recognition in drug design: preliminary application of free energy derivatives to inhibition of a malarial cysteine protease. <i>Journal of Molecular Recognition</i> , <b>1996</b> , 9, 103-122	2.6	4
13	CaspNeuroD: a knowledgebase of predicted caspase cleavage sites in human proteins related to neurodegenerative diseases. <i>Database: the Journal of Biological Databases and Curation</i> , <b>2016</b> , 2016,	5	4
12	Letter to the Editor: Caspase cleavage sites in the human proteome: CaspDB, a database of predicted substrates. <i>Apoptosis: an International Journal on Programmed Cell Death</i> , <b>2015</b> , 20, 421	5.4	3
11	Interaction of the cryptic fragment of myelin basic protein with mitochondrial voltage-dependent anion-selective channel-1 affects cell energy metabolism. <i>Biochemical Journal</i> , <b>2018</b> , 475, 2355-2376	3.8	3
10	S-Nitrosylation of p62 Inhibits Autophagic Flux to Promote $\alpha$ -Synuclein Secretion and Spread in Parkinson's Disease and Lewy Body Dementia.. <i>Journal of Neuroscience</i> , <b>2022</b> ,	6.6	3
9	Application of the Free Energy Calculations to Study Drug-enzyme and Drug-dna Complexes. <i>Molecular Simulation</i> , <b>2002</b> , 28, 173-186	2	2
8	Hydration of Benzoic Acid in Benzene Solution. <i>Zeitschrift Fur Physikalische Chemie</i> , <b>1992</b> , 177, 63-74	3.1	2
7	Peptide Sequence Region That is Essential for the Interactions of the Enterotoxigenic Bacteroides fragilis Metalloproteinase II with E-cadherin <b>2014</b> , 1, 3-14		2
6	A Note on the Potential BCG Vaccination $\square$ COVID-19 Molecular Link. <i>Coronaviruses</i> , <b>2020</b> , 1, 4-6	1.5	2
5	Quantitative profiling of protease specificity. <i>PLoS Computational Biology</i> , <b>2021</b> , 17, e1008101	5	2
4	Toxoplasma gondii serine hydrolases regulate parasite lipid mobilization during growth and replication within the host. <i>Cell Chemical Biology</i> , <b>2021</b> , 28, 1501-1513.e5	8.2	0
3	Stress tensor and constant pressure simulation for polarizable Gaussian multipole model.. <i>Journal of Chemical Physics</i> , <b>2022</b> , 156, 114114	3.9	0
2	Interactions between motor domains in kinesin-14 Ncd - a molecular dynamics study. <i>Biochemical Journal</i> , <b>2019</b> , 476, 2449-2462	3.8	
1	Identifying protease cleavage sites by label-free mass spectrometry. <i>FASEB Journal</i> , <b>2010</b> , 24, 905.4	0.9	