Carmay Lim

List of Publications by Citations

173 papers	6,418 citations	43 h-index	73 g-index
183 ext. papers	7,114 ext. citations	9.3 avg, IF	6.19 L-index

#	Paper	IF	Citations
173	Principles governing Mg, Ca, and Zn binding and selectivity in proteins. *Chemical Reviews*, **2003**, 103, 773-88	68.1	373
172	Absolute pKa calculations with continuum dielectric methods. *The Journal of Physical Chemistry*, **1991**, 95, 5610-5620		370
171	Competition among metal ions for protein binding sites: determinants of metal ion selectivity in proteins. *Chemical Reviews*, **2014**, 114, 538-56	68.1	247
170	Metal binding affinity and selectivity in metalloproteins: insights from computational studies. *Annual Review of Biophysics*, **2008**, 37, 97-116	21.1	177
169	Ring Strain Energies from ab Initio Calculations. *Journal of the American Chemical Society*, **1998**, 120, 4450-4458	16.4	175
168	Tetrahedral vs Octahedral Zinc Complexes with Ligands of Biological Interest: A DFT/CDM Study. *Journal of the American Chemical Society*, **2000**, 122, 11146-11153	16.4	174
167	First-second shell interactions in metal binding sites in proteins: a PDB survey and DFT/CDM calculations. *Journal of the American Chemical Society*, **2003**, 125, 3168-80	16.4	168
166	Competitive Binding in Magnesium Coordination Chemistry: Water versus Ligands of Biological Interest. *Journal of the American Chemical Society*, **1999**, 121, 7665-7673	16.4	130
165	Zn protein simulations including charge transfer and local polarization effects. *Journal of the American Chemical Society*, **2005**, 127, 4921-9	16.4	116
164	Empirical force fields for biologically active divalent metal cations in water. *Journal of Physical Chemistry A*, **2006**, 110, 691-9	2.8	115
163	Theory of Ionic Hydration: Insights from Molecular Dynamics Simulations and Experiment. *Journal of Physical Chemistry B*, **1999**, 103, 7958-7968	3.4	113
162	Monodentate versus Bidentate Carboxylate Binding in Magnesium and Calcium Proteins: What Are the Basic Principles?. *Journal of Physical Chemistry B*, **2004**, 108, 4546-4557	3.4	100
161	Effect of carboxylate-binding mode on metal binding/selectivity and function in proteins. *Accounts of Chemical Research*, **2007**, 40, 85-93	24.3	99
160	Atom-surface scattering dynamics at hyperthermal energies. *Journal of Chemical Physics*, **1987**, 87, 1796-1807	3.9	99
159	How Molecular Size Impacts RMSD Applications in Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 1518-1524	6.4	98
158	Free energy decomposition of protein-protein interactions. *Biophysical Journal*, **2001**, 81, 737-50	2.9	97
157	Factors governing the metal coordination number in metal complexes from Cambridge Structural Database analyses. *Journal of Physical Chemistry B*, **2006**, 110, 1889-95	3.4	93

156	Factors governing the protonation state of cysteines in proteins: an Ab initio/CDM study. *Journal of the American Chemical Society*, **2002**, 124, 6759-66	16.4	89
155	Factors governing metal-ligand distances and coordination geometries of metal complexes. *Journal of Physical Chemistry B*, **2009**, 113, 2952-60	3.4	88
154	Physical basis of structural and catalytic Zn-binding sites in proteins. *Journal of Molecular Biology*, **2008**, 379, 545-53	6.5	88
153	Determinants of K+ vs Na+ selectivity in potassium channels. *Journal of the American Chemical Society*, **2009**, 131, 8092-101	16.4	80
152	An azido-BODIPY probe for glycosylation: initiation of strong fluorescence upon triazole formation. *Journal of the American Chemical Society*, **2014**, 136, 9953-61	16.4	76
151	A simple biophysical model emulates budding yeast chromosome condensation. *ELife*, **2015**, 4, e05565	8.9	71
150	Competition between Li+ and Mg2+ in metalloproteins. Implications for lithium therapy. *Journal of the American Chemical Society*, **2011**, 133, 9506-15	16.4	67
149	Nonexistence of dianionic pentacovalent intermediates in an ab initio study of the base-catalyzed hydrolysis of ethylene phosphate. *Journal of the American Chemical Society*, **1990**, 112, 5872-5873	16.4	65
148	Factors governing the Na(+) vs K(+) selectivity in sodium ion channels. *Journal of the American Chemical Society*, **2010**, 132, 2321-32	16.4	64
147	Metal Selectivity in Metalloproteins:Zn2+vs Mg2+. *Journal of Physical Chemistry B*, **2001**, 105, 4446-4452	3.4	63
146	A combined experimental and theoretical study of divalent metal ion selectivity and function in proteins: application to E. coli ribonuclease H1. *Journal of the American Chemical Society*, **2003**, 125, 9318-28	16.4	61
145	Polarization-consistent versus correlation-consistent basis sets in predicting molecular and spectroscopic properties. *Journal of Physical Chemistry A*, **2007**, 111, 1927-32	2.8	55
144	Dianionic pentacoordinate species in the base-catalyzed hydrolysis of ethylene and dimethyl phosphate. *Journal of the American Chemical Society*, **1991**, 113, 4353-4355	16.4	55
143	Factors governing the substitution of La3+ for Ca2+ and Mg2+ in metalloproteins: a DFT/CDM study. *Journal of the American Chemical Society*, **2005**, 127, 4091-103	16.4	53
142	A DFT/CDM Study of metal-carboxylate interactions in metalloproteins: factors governing the maximum number of metal-bound carboxylates. *Journal of the American Chemical Society*, **2006**, 128, 1553-61	16.4	53
141	Metal Binding in Proteins: The Effect of the Dielectric Medium. *Journal of Physical Chemistry B*, **2000**, 104, 3692-3694	3.4	52
140	Molecular dynamics simulation of E. coli ribonuclease H1 in solution: correlation with NMR and X-ray data and insights into biological function. *Journal of Molecular Biology*, **1995**, 254, 771-92	6.5	52
139	Discovering structural motifs using a structural alphabet: application to magnesium-binding sites. *BMC Bioinformatics*, **2007**, 8, 106	3.6	51

138	Exploring the dynamic information content of a protein NMR structure: comparison of a molecular dynamics simulation with the NMR and X-ray structures of Escherichia coli ribonuclease HI. *Proteins: Structure, Function and Bioinformatics*, **1999**, 36, 87-110	4.2	51
137	Accuracy and precision of NMR relaxation experiments and MD simulations for characterizing protein dynamics. *Proteins: Structure, Function and Bioinformatics*, **1997**, 28, 481-493	4.2	49
136	Structural analysis of disease-related TDP-43 D169G mutation: linking enhanced stability and caspase cleavage efficiency to protein accumulation. *Scientific Reports*, **2016**, 6, 21581	4.9	47
135	Simulation analysis of structures on the reaction pathway of RNAse A. *Journal of the American Chemical Society*, **1990**, 112, 3826-3831	16.4	47
134	Trajectory studies of hyperthermal Xe scattering from GaAs(110). *Journal of Chemical Physics*, **1987**, 87, 1808-1816	3.9	47
133	Ion selectivity strategies of sodium channel selectivity filters. *Accounts of Chemical Research*, **2014**, 47, 3580-7	24.3	46
132	Force fields including charge transfer and local polarization effects: Application to proteins containing multi/heavy metal ions. *Journal of Computational Chemistry*, **2009**, 30, 191-202	3.5	44
131	Factors controlling the reactivity of zinc finger cores. *Journal of the American Chemical Society*, **2011**, 133, 8691-703	16.4	43
130	Importance of metal hydration on the selectivity of Mg2+ versus Ca2+ in magnesium ion channels. *Journal of the American Chemical Society*, **2013**, 135, 17200-8	16.4	42
129	Factors governing the metal coordination number in isolated group IA and IIA metal hydrates. *Inorganic Chemistry*, **2006**, 45, 4811-9	5.1	42
128	Factors governing the protonation state of Zn-bound histidine in proteins: a DFT/CDM study. *Journal of the American Chemical Society*, **2004**, 126, 2602-12	16.4	42
127	Modeling Zn2+Cysteinate Complexes in Proteins. *Journal of Physical Chemistry B*, **2001**, 105, 10709-10714	3.4	42
126	Incremental Binding Free Energies in Mg2+ Complexes: A DFT Study. *Journal of Physical Chemistry A*, **1999**, 103, 8093-8100	2.8	42
125	Structural Characterization of the Phosphotyrosine Binding Region of a High-Affinity SH2 DomainPhosphopeptide Complex by Molecular Dynamics Simulation and Chemical Shift Calculations. *Journal of the American Chemical Society*, **1996**, 118, 11265-11277	16.4	42
124	Selectivity Mechanism of the Voltage-gated Proton Channel, HV1. *Scientific Reports*, **2015**, 5, 10320	4.9	41
123	Computational studies of the coordination stereochemistry, bonding, and metal selectivity of mercury. *Journal of Physical Chemistry A*, **2006**, 110, 452-62	2.8	41
122	Factors Governing the Enhanced Reactivity of Five-Membered Cyclic Phosphate Esters. *Journal of the American Chemical Society*, **1998**, 120, 2156-2167	16.4	41
121	Concerted hydroxyl ion attack and pseudorotation in the base-catalyzed hydrolysis of methyl ethylene phosphate. *The Journal of Physical Chemistry*, **1992**, 96, 5217-5219		41

120	Multi-targeting of functional cysteines in multiple conserved SARS-CoV-2 domains by clinically safe Zn-ejectors. *Chemical Science*, **2020**, 11, 9904-9909	9.4	40
119	Competition among Ca2+, Mg2+, and Na+ for model ion channel selectivity filters: determinants of ion selectivity. *Journal of Physical Chemistry B*, **2012**, 116, 10703-14	3.4	38
118	Predicting RNA-binding sites from the protein structure based on electrostatics, evolution and geometry. *Nucleic Acids Research*, **2008**, 36, e29	20.1	38
117	Endocyclic and exocyclic cleavage of phosphorane monoanion: a detailed mechanism of the RNase A transphosphorylation step. *Journal of the American Chemical Society*, **1992**, 114, 7245-7252	16.4	38
116	New insights into the base-catalyzed hydrolysis of methyl ethylene phosphate. *The Journal of Physical Chemistry*, **1993**, 97, 6212-6219		37
115	DR_bind: a web server for predicting DNA-binding residues from the protein structure based on electrostatics, evolution and geometry. *Nucleic Acids Research*, **2012**, 40, W249-56	20.1	34
114	Structural and Physical Basis for Anti-IgE Therapy. *Scientific Reports*, **2015**, 5, 11581	4.9	33
113	Mononuclear versus binuclear metal-binding sites: metal-binding affinity and selectivity from PDB survey and DFT/CDM calculations. *Journal of the American Chemical Society*, **2008**, 130, 3844-52	16.4	33
112	The Significance of Electrostatic Effects in Phospho-Ester Hydrolysis. *Journal of the American Chemical Society*, **1994**, 116, 3922-3931	16.4	33
111	A new interpretation of the effective Born radius from simulation and experiment. *Chemical Physics Letters*, **1999**, 310, 225-228	2.5	32
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109	An ab Initio Study of Nucleophilic Attack of Trimethyl Phosphate: Factors Influencing Site Reactivity. *Journal of Physical Chemistry A*, **1997**, 101, 8706-8713	2.8	30
108	Dynamic Model of Lignin Growing in Restricted Spaces. *Macromolecules*, **1995**, 28, 370-376	5.5	30
107	Metal Binding and Selectivity in Zinc Proteins. *Journal of the Chinese Chemical Society*, **2003**, 50, 1093-1102	1.5	28
106	Structural Basis for the Magnesium-Dependent Activation and Hexamerization of the Lon AAA+ Protease. *Structure*, **2016**, 24, 676-686	5.2	28
105	Preferred Hydrogen-Bonding Partners of Cysteine: Implications for Regulating Cys Functions. *Journal of Physical Chemistry B*, **2016**, 120, 10288-10296	3.4	27
104	Differential effects of the Zn-His-Bkb vs Zn-His-[Asp/Glu] triad on Zn-core stability and reactivity. *Journal of the American Chemical Society*, **2005**, 127, 11336-47	16.4	27
103	Representing an Infinite Solvent System with a Rectangular Finite System Using Image Charges. *Journal of Physical Chemistry B*, **2002**, 106, 2973-2982	3.4	26

102	Using an Old Drug to Target a New Drug Site: Application of Disulfiram to Target the Zn-Site in HCV NS5A Protein. *Journal of the American Chemical Society*, **2016**, 138, 3856-62	16.4	26
101	How Native and Alien Metal Cations Bind ATP: Implications for Lithium as a Therapeutic Agent. *Scientific Reports*, **2017**, 7, 42377	4.9	25
100	Sequence-motif detection of NAD(P)-binding proteins: discovery of a unique antibacterial drug target. *Scientific Reports*, **2014**, 4, 6471	4.9	24
99	Factors governing loss and rescue of DNA binding upon single and double mutations in the p53 core domain. *Nucleic Acids Research*, **2002**, 30, 1563-74	20.1	24
98	Reducing the error due to the uncertainty in the Born radius in continuum dielectric calculations. *The Journal of Physical Chemistry*, **1994**, 98, 692-695		24
97	Nonequilibrium effects in chemical kinetics. Straight-line paths for homonuclear diatomic dissociation-recombination process. *The Journal of Physical Chemistry*, **1983**, 87, 2683-2699		23
96	Molecular dynamics of nonequilibrium infrequent events: Laser-induced desorption from surfaces. *Journal of Chemical Physics*, **1986**, 85, 7423-7433	3.9	22
95	How Pb Binds and Modulates Properties of Ca-Signaling Proteins. *Inorganic Chemistry*, **2018**, 57, 14798-14809	5.1	22
94	Soluble klotho regulates TRPC6 calcium signaling lipid rafts, independent of the FGFR-FGF23 pathway. *FASEB Journal*, **2019**, 33, 9182-9193	0.9	21
93	Modeled structural basis for the recognition of α-2-3-sialyllactose by soluble Klotho. *FASEB Journal*, **2017**, 31, 3574-3586	0.9	20
92	Relationship between Enzyme/Substrate Properties and Enzyme Efficiency in Hydrolases. *ACS Catalysis*, **2015**, 5, 5877-5887	13.1	20
91	Evolution of eukaryotic ion channels: principles underlying the conversion of Ca2+-selective to Na+-selective channels. *Journal of the American Chemical Society*, **2014**, 136, 3553-9	16.4	20
90	Metal-binding affinity and selectivity of nonstandard natural amino acid residues from DFT/CDM calculations. *Journal of Physical Chemistry B*, **2009**, 113, 11754-64	3.4	20
89	All-electron calculations of the nucleation structures in metal-induced zinc-finger folding: role of the Peptide backbone. *Journal of the American Chemical Society*, **2007**, 129, 12497-504	16.4	20
88	Synergistic Inhibition of SARS-CoV-2 Replication Using Disulfiram/Ebselen and Remdesivir. *ACS Pharmacology and Translational Science*, **2021**, 4, 898-907	5.9	20
87	A structural-alphabet-based strategy for finding structural motifs across protein families. *Nucleic Acids Research*, **2010**, 38, e150	20.1	19
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85	Oxyanion selectivity in sulfate and molybdate transport proteins: an ab initio/CDM study. *Journal of the American Chemical Society*, **2004**, 126, 10296-305	16.4	19

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83	Ion selectivity in the selectivity filters of acid-sensing ion channels. *Scientific Reports*, **2015**, 5, 7864	4.9	18
82	Predicting DNA-binding amino acid residues from electrostatic stabilization upon mutation to Asp/Glu and evolutionary conservation. *Proteins: Structure, Function and Bioinformatics*, **2007**, 67, 671-80	4.2	18
81	Solvation free energies of polar molecular solutes: Application of the two-sphere Born radius in continuum models of solvation. *Journal of Chemical Physics*, **2001**, 114, 889	3.9	18
80	Differential role of the protein matrix on the binding of a catalytic aspartate to Mg2+ vs Ca2+: application to ribonuclease H. *Journal of the American Chemical Society*, **2013**, 135, 6541-8	16.4	17
79	Factors Controlling the Role of Zn and Reactivity of Zn-bound Cysteines in Proteins: Application to Drug Target Discovery. *Journal of the Chinese Chemical Society*, **2014**, 61, 142-150	1.5	17
78	Mechanism of DNA-binding loss upon single-point mutation in p53. *Journal of Biosciences*, **2007**, 32, 827-39	2.3	17
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75	Factors controlling the selectivity for Na(+) over Mg(2+) in sodium transporters and enzymes. *Physical Chemistry Chemical Physics*, **2016**, 18, 16986-97	3.6	15
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71	Linking distinct conformations of nicotinamide adenine dinucleotide with protein fold/function. *Journal of Physical Chemistry B*, **2011**, 115, 7932-9	3.4	15
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66	Reformulation of Maxwell's equations to incorporate near-solute solvent structure. *Journal of Physical Chemistry B*, **2008**, 112, 10791-4	3.4	13
65	Design, synthesis, and SAR of novel carbapenem antibiotics with high stability to Xanthomonas maltophilia oxyiminocephalosporinase type II. *Journal of Medicinal Chemistry*, **2000**, 43, 3632-40	8.3	13
64	Internal Motions in the Molecular Tumbling Regime. Effect on NMR Dipolar Cross-Relaxation and Interproton Distance Determination. *The Journal of Physical Chemistry*, **1994**, 98, 8264-8273		13
63	The effect of vibrational-rotational disequilibrium on the rate constant for an atom-transfer reaction. *The Journal of Physical Chemistry*, **1986**, 90, 2616-2634		13
62	How the Local Environment of Functional Sites Regulates Protein Function. *Journal of the American Chemical Society*, **2020**, 142, 9861-9871	16.4	12
61	Strategies to model the near-solute solvent molecular density/polarization. *Journal of Computational Chemistry*, **2009**, 30, 700-9	3.5	12
60	Redesign of high-affinity nonspecific nucleases with altered sequence preference. *Journal of the American Chemical Society*, **2009**, 131, 17345-53	16.4	12
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58	Positive charge at position 549 is essential for phosphatidylinositol 4,5-bisphosphate-hydrolyzing but not phosphatidylinositol-hydrolyzing activities of human phospholipase C delta1. *Journal of Biological Chemistry*, **1996**, 271, 24505-16	5.4	12
57	Simulation Analysis of the Binding Interactions in the RNase A/3RUMP Enzyme-Product Complex as a Function of pH. *Journal of the American Chemical Society*, **1994**, 116, 2591-2599	16.4	12
56	Quantum-chemistry based calibration of the alkali metal cation series (Li(+)-Cs(+)) for large-scale polarizable molecular mechanics/dynamics simulations. *Journal of Computational Chemistry*, **2015**, 36, 285-302	3.5	11
55	The effect of metal binding on the characteristic infrared band intensities of ligands of biological interest. *Journal of Molecular Structure*, **2012**, 1009, 83-88	3.4	11
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53	Factors controlling the mechanism of NAD(+) non-redox reactions. *Journal of the American Chemical Society*, **2010**, 132, 16533-43	16.4	11
52	Combined experimental and theoretical study of long-range interactions modulating dimerization and activity of yeast geranylgeranyl diphosphate synthase. *Journal of the American Chemical Society* , **2009**, 131, 4051-62	16.4	11
51	Competition between protein ligands and cytoplasmic inorganic anions for the metal cation: a DFT/CDM study. *Journal of the American Chemical Society*, **2006**, 128, 10541-8	16.4	11
50	Study of mixture effects in the nonequilibrium kinetics of homonuclear diatomic dissociation and recombination. *The Journal of Physical Chemistry*, **1984**, 88, 778-792		11
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47	Incorporating Nonlinear Solvent Response in Continuum Dielectric Models Using a Two-Sphere Description of the Born Radius. *Journal of Physical Chemistry A*, **2001**, 105, 5030-5036	2.8	10
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45	Ran pathway-independent regulation of mitotic Golgi disassembly by Importin-□*Nature Communications*, **2019**, 10, 4307	17.4	9
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43	Hidden relationship between conserved residues and locally conserved phosphate-binding structures in NAD(P)-binding proteins. *Journal of Physical Chemistry B*, **2012**, 116, 5644-52	3.4	9
42	Arrangement of 3D structural motifs in ribosomal RNA. *Nucleic Acids Research*, **2010**, 38, 3512-22	20.1	9
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40	Sensitive and Specific Cadmium Biosensor Developed by Reconfiguring Metal Transport and Leveraging Natural Gene Repositories. *ACS Sensors*, **2021**, 6, 995-1002	9.2	8
39	How Native and Non-Native Cations Bind and Modulate the Properties of GTP/ATP. *Journal of Chemical Theory and Computation*, **2018**, 14, 3311-3320	6.4	8
38	Conserved structural motif for recognizing nicotinamide adenine dinucleotide in poly(ADP-ribose) polymerases and ADP-ribosylating toxins: implications for structure-based drug design. *Journal of Medicinal Chemistry*, **2010**, 53, 4038-49	8.3	7
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30	Benchmarking polarizable and non-polarizable force fields for Ca-peptides against a comprehensive QM dataset. *Journal of Chemical Physics*, **2020**, 153, 144102	3.9	5
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26	Factors Governing the Different Functions of Zn-Sites with Identical Ligands in Proteins. *Journal of Chemical Information and Modeling*, **2019**, 59, 3946-3954	6.1	4
25	Free and Bound Therapeutic Lithium in Brain Signaling. *Accounts of Chemical Research*, **2019**, 52, 2960-2970	24.3	4
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19	Factors Governing the Bridging Water Protonation State in Polynuclear Mg(2+) Proteins. *Journal of Physical Chemistry B*, **2016**, 120, 1759-70	3.4	3
18	Comparative effects of human Ig alpha and Ig beta in inducing autoreactive antibodies against B cells in mice. *Journal of Immunology*, **2003**, 170, 1158-66	5.3	3
17	Configurational Entropy of Proteins: Covariance Matrix versus Cumulative Distribution Calculations. *Journal of the Chinese Chemical Society*, **2004**, 51, 1209-1219	1.5	3
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14	Sensitivity of Functional Loop Conformations on Long-Range Electrostatics: Implications for M20 Loop Dynamics in Dihydrofolate Reductase. *Journal of Chemical Theory and Computation*, **2020**, 16, 2028-2033	6.4	2
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8	Preparing a human membrane and secreted protein-enriched cDNA library using PCR primers derived from a genomic database. *Nucleic Acids Research*, **2001**, 29, E114	20.1	1
7	Conformational Distribution of a Tetrapeptide in Solution Using a Combined Random Search and Continuum Dielectric Approach. *The Journal of Physical Chemistry*, **1994**, 98, 12805-12814		1
6	Gene Silencing Mechanisms Revealed by Dynamics of Guide, Target, and Duplex Binding to Argonaute. *Journal of Chemical Theory and Computation*, **2020**, 16, 688-699	6.4	1
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