

S Gnanakaran

List of Publications by Year in descending order

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101
papers

7,654
citations

61984

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58581

82
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113
all docs

113
docs citations

113
times ranked

11291
citing authors

#	ARTICLE	IF	CITATIONS
1	Machine learning-driven multiscale modeling reveals lipid-dependent dynamics of RAS signaling proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	7.1	44
2	Predictive Rules of Efflux Inhibition and Avoidance in <i>Pseudomonas aeruginosa</i> . <i>MBio</i> , 2021, 12, .	4.1	28
3	Development of Martini 2.2 parameters for <i>N</i> -glycans: a case study of the HIV-1 Env glycoprotein dynamics. <i>Glycobiology</i> , 2021, 31, 787-799.	2.5	7
4	Microscopic Approach to Intrinsic Antibiotic Resistance. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3114-3118.	2.6	5
5	Unveiling the Dynamics of KRAS4b on Lipid Model Membranes. <i>Journal of Membrane Biology</i> , 2021, 254, 201-216.	2.1	6
6	Effects of pH on an IDP conformational ensemble explored by molecular dynamics simulation. <i>Biophysical Chemistry</i> , 2021, 271, 106552.	2.8	18
7	The SARS-CoV-2 Spike variant D614G favors an open conformational state. <i>Science Advances</i> , 2021, 7, .	10.3	156
8	Molecular characterization of the outer membrane of <i>Pseudomonas aeruginosa</i> . <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020, 1862, 183151.	2.6	28
9	Visualization of the HIV-1 Env glycan shield across scales. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 28014-28025.	7.1	57
10	Uncovering a membrane-distal conformation of KRAS available to recruit RAF to the plasma membrane. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 24258-24268.	7.1	34
11	Quantification of the Resilience and Vulnerability of HIV-1 Native Glycan Shield at Atomistic Detail. <i>IScience</i> , 2020, 23, 101836.	4.1	11
12	Graph-Directed Approach for Downselecting Toxins for Experimental Structure Determination. <i>Marine Drugs</i> , 2020, 18, 256.	4.6	4
13	Machine Learning Algorithm Identifies an Antibiotic Vocabulary for Permeating Gram-Negative Bacteria. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2838-2847.	5.4	21
14	Emergence of SARS-CoV-2 through recombination and strong purifying selection. <i>Science Advances</i> , 2020, 6, .	10.3	307
15	Anionic Lipids Impact RAS-Binding Site Accessibility and Membrane Binding Affinity of CRAF RBD-CRD. <i>Biophysical Journal</i> , 2020, 119, 525-538.	0.5	13
16	Computing long time scale biomolecular dynamics using quasi-stationary distribution kinetic Monte Carlo (QSD-KMC). <i>Journal of Chemical Physics</i> , 2019, 151, 074109.	3.0	4
17	Combinatorial diversity of Syk recruitment driven by its multivalent engagement with $Fc\mu R1^3$. <i>Molecular Biology of the Cell</i> , 2019, 30, 2331-2347.	2.1	11
18	Unsupervised Machine Learning for Analysis of Phase Separation in Ternary Lipid Mixture. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6343-6357.	5.3	18

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19	Snails In Silico: A Review of Computational Studies on the Conopeptides. <i>Marine Drugs</i> , 2019, 17, 145.	4.6	21
20	Biophysical Characterization of a Nanodisc with and without BAX: An Integrative Study Using Molecular Dynamics Simulations and Cryo-EM. <i>Structure</i> , 2019, 27, 988-999.e4.	3.3	19
21	HIV-1 Neutralizing Antibody Signatures and Application to Epitope-Targeted Vaccine Design. <i>Cell Host and Microbe</i> , 2019, 25, 59-72.e8.	11.0	124
22	Sequence- and structure-based computational analyses of Gram-negative tripartite efflux pumps in the context of bacterial membranes. <i>Research in Microbiology</i> , 2018, 169, 414-424.	2.1	6
23	Capturing Phase Behavior of Ternary Lipid Mixtures with a Refined Martini Coarse-Grained Force Field. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6050-6062.	5.3	63
24	Molecular recognition of RAS/RAF complex at the membrane: Role of RAF cysteine-rich domain. <i>Scientific Reports</i> , 2018, 8, 8461.	3.3	71
25	Membrane perturbing properties of toxin mycolactone from <i>Mycobacterium ulcerans</i> . <i>PLoS Computational Biology</i> , 2018, 14, e1005972.	3.2	28
26	Switch Loop Flexibility Affects Substrate Transport of the AcrB Efflux Pump. <i>Journal of Molecular Biology</i> , 2017, 429, 3863-3874.	4.2	33
27	Dynamics of Intact MexAB-OprM Efflux Pump: Focusing on the MexA-OprM Interface. <i>Scientific Reports</i> , 2017, 7, 16521.	3.3	30
28	Effect of Glycosylation on an Immunodominant Region in the V1V2 Variable Domain of the HIV-1 Envelope gp120 Protein. <i>PLoS Computational Biology</i> , 2016, 12, e1005094.	3.2	17
29	Dynamics of a chlorophyll dimer in collective and local thermal environments. <i>Journal of Mathematical Chemistry</i> , 2016, 54, 866-917.	1.5	15
30	Broadly targeted CD8 ⁺ T cell responses restricted by major histocompatibility complex E. <i>Science</i> , 2016, 351, 714-720.	12.6	260
31	The eighth q-bio conference: meeting report and special issue preface. <i>Physical Biology</i> , 2015, 12, 060401.	1.8	0
32	Longitudinal Antigenic Sequences and Sites from Intra-Host Evolution (LASSIE) Identifies Immune-Selected HIV Variants. <i>Viruses</i> , 2015, 7, 5443-5475.	3.3	26
33	Membrane-Mediated Regulation of the Intrinsically Disordered CD3 ζ Cytoplasmic Tail of the TCR. <i>Biophysical Journal</i> , 2015, 108, 2481-2491.	0.5	21
34	MARTINI Coarse-Grained Model for Crystalline Cellulose Microfibers. <i>Journal of Physical Chemistry B</i> , 2015, 119, 465-473.	2.6	54
35	A data-driven approach to modeling the tripartite structure of multidrug resistance efflux pumps. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 46-65.	2.6	31
36	Permeability Barrier of Gram-Negative Cell Envelopes and Approaches To Bypass It. <i>ACS Infectious Diseases</i> , 2015, 1, 512-522.	3.8	442

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37	Sodium Ion Interactions with Aqueous Glucose: Insights from Quantum Mechanics, Molecular Dynamics, and Experiment. <i>Journal of Physical Chemistry B</i> , 2014, 118, 1990-2000.	2.6	49
38	The Seventh q-bio Conference: meeting report and preface. <i>Physical Biology</i> , 2014, 11, 040301.	1.8	1
39	Systems Level Study of Bacterial Multi-Drug Resistance from Efflux Machinery. <i>Biophysical Journal</i> , 2014, 106, 791a.	0.5	0
40	Common processes drive the thermochemical pretreatment of lignocellulosic biomass. <i>Green Chemistry</i> , 2014, 16, 63-68.	9.0	198
41	Structure and dynamics of a complex of cellulose with EDA: insights into the action of amines on cellulose. <i>Cellulose</i> , 2013, 20, 1563-1571.	4.9	18
42	Polyelectrolyte multilayers as a platform for pH-responsive lipid bilayers. <i>Soft Matter</i> , 2013, 9, 8938.	2.7	17
43	Deducing conformational variability of intrinsically disordered proteins from infrared spectroscopy with Bayesian statistics. <i>Chemical Physics</i> , 2013, 422, 143-155.	1.9	13
44	Taste of Sugar at the Membrane: Thermodynamics and Kinetics of the Interaction of a Disaccharide with Lipid Bilayers. <i>Biophysical Journal</i> , 2013, 104, 622-632.	0.5	22
45	Co-evolution of a broadly neutralizing HIV-1 antibody and founder virus. <i>Nature</i> , 2013, 496, 469-476.	27.8	961
46	Sodium chloride interaction with solvated and crystalline cellulose: sodium ion affects the cellotetraose molecule and the cellulose fibril in aqueous solution. <i>Cellulose</i> , 2013, 20, 2695-2702.	4.9	14
47	A Mechanistic Understanding of Allosteric Immune Escape Pathways in the HIV-1 Envelope Glycoprotein. <i>PLoS Computational Biology</i> , 2013, 9, e1003046.	3.2	53
48	Viral Escape from Neutralizing Antibodies in Early Subtype A HIV-1 Infection Drives an Increase in Autologous Neutralization Breadth. <i>PLoS Pathogens</i> , 2013, 9, e1003173.	4.7	55
49	Special section dedicated to The Sixth q-bio Conference: meeting report and preface. <i>Physical Biology</i> , 2013, 10, 030301.	1.8	2
50	Increased enzyme binding to substrate is not necessary for more efficient cellulose hydrolysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 10922-10927.	7.1	131
51	Plasma IgG to Linear Epitopes in the V2 and V3 Regions of HIV-1 gp120 Correlate with a Reduced Risk of Infection in the RV144 Vaccine Efficacy Trial. <i>PLoS ONE</i> , 2013, 8, e75665.	2.5	214
52	The Fifth Annual q-bio Conference on Cellular Information Processing. <i>Physical Biology</i> , 2012, 9, 050201.	1.8	0
53	Temperature Dependence of Water Interactions with the Amide Carbonyls of α -Helices. <i>Biochemistry</i> , 2012, 51, 5293-5299.	2.5	25
54	Coarse-Grained Model for the Interconversion between Native and Liquid Ammonia-Treated Crystalline Cellulose. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8031-8037.	2.6	27

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55	Characterization of a Disordered Protein during Micellation: Interactions of $\hat{\pm}$ -Synuclein with Sodium Dodecyl Sulfate. <i>Journal of Physical Chemistry B</i> , 2012, 116, 4417-4424.	2.6	15
56	A coarse-grained model for synergistic action of multiple enzymes on cellulose. <i>Biotechnology for Biofuels</i> , 2012, 5, 55.	6.2	39
57	Identification of Minimally Interacting Modules in an Intrinsically Disordered Protein. <i>Biophysical Journal</i> , 2012, 103, 748-757.	0.5	26
58	Sequential exposure to specific antibody escape mutations may program neutralization breadth during subtype A HIV-1 infection. <i>Retrovirology</i> , 2012, 9, .	2.0	0
59	Understanding the interaction of Lipoarabinomannan with membrane mimetic architectures. <i>Tuberculosis</i> , 2012, 92, 38-47.	1.9	22
60	Exploring new strategies for cellulosic biofuels production. <i>Energy and Environmental Science</i> , 2011, 4, 3820.	30.8	79
61	Assisted Peptide Folding by Surface Pattern Recognition. <i>Biophysical Journal</i> , 2011, 100, 1306-1315.	0.5	18
62	Restructuring the Crystalline Cellulose Hydrogen Bond Network Enhances Its Depolymerization Rate. <i>Journal of the American Chemical Society</i> , 2011, 133, 11163-11174.	13.7	321
63	Probing the Early Events Associated with Liquid Ammonia Pretreatment of Native Crystalline Cellulose. <i>Journal of Physical Chemistry B</i> , 2011, 115, 9782-9788.	2.6	33
64	Theoretical Study of the Remarkably Diverse Linkages in Lignin. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2660-2666.	4.6	335
65	Insights into Hydrogen Bonding and Stacking Interactions in Cellulose. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14191-14202.	2.5	122
66	Quantum Chemical Study of Carbohydrate-Phospholipid Interactions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12826-12840.	2.5	7
67	Identification of amino acid substitutions associated with neutralization phenotype in the human immunodeficiency virus type-1 subtype C gp120. <i>Virology</i> , 2011, 409, 163-174.	2.4	18
68	Neutron crystallographic and molecular dynamics studies of the structure of ammonia-cellulose I: rearrangement of hydrogen bonding during the treatment of cellulose with ammonia. <i>Cellulose</i> , 2011, 18, 191-206.	4.9	39
69	Converging on an HIV Vaccine. <i>Science</i> , 2011, 333, 1589-1590.	12.6	17
70	The B Cell Response Is Redundant and Highly Focused on V1V2 during Early Subtype C Infection in a Zambian Seroconverter. <i>Journal of Virology</i> , 2011, 85, 905-915.	3.4	66
71	Quantifying Intramolecular Binding in Multivalent Interactions: A Structure-Based Synergistic Study on Grb2-Sos1 Complex. <i>PLoS Computational Biology</i> , 2011, 7, e1002192.	3.2	17
72	Epitopes Immediately below the Base of the V3 Loop of gp120 as Targets for the Initial Autologous Neutralizing Antibody Response in Two HIV-1 Subtype B-Infected Individuals. <i>Journal of Virology</i> , 2011, 85, 9286-9299.	3.4	24

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73	Recurrent Signature Patterns in HIV-1 B Clade Envelope Glycoproteins Associated with either Early or Chronic Infections. <i>PLoS Pathogens</i> , 2011, 7, e1002209.	4.7	114
74	A Signature in HIV-1 Envelope Leader Peptide Associated with Transition from Acute to Chronic Infection Impacts Envelope Processing and Infectivity. <i>PLoS ONE</i> , 2011, 6, e23673.	2.5	54
75	Subtype-specific conservation of isoleucine 309 in the envelope V3 domain is linked to immune evasion in subtype C HIV-1 infection. <i>Virology</i> , 2010, 404, 59-70.	2.4	30
76	In silicostudies of crystalline cellulose and its degradation by enzymes. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1184-1188.	2.5	25
77	Genetic Signatures in the Envelope Glycoproteins of HIV-1 that Associate with Broadly Neutralizing Antibodies. <i>PLoS Computational Biology</i> , 2010, 6, e1000955.	3.2	78
78	Nature and Kinetic Analysis of Carbon ¹³ Carbon Bond Fragmentation Reactions of Cation Radicals Derived from SET-Oxidation of Lignin Model Compounds. <i>Journal of Organic Chemistry</i> , 2010, 75, 6549-6562.	3.2	88
79	Appreciating HIV Type 1 Diversity: Subtype Differences in Env. <i>AIDS Research and Human Retroviruses</i> , 2009, 25, 237-248.	1.1	69
80	Escape from Autologous Neutralizing Antibodies in Acute/Early Subtype C HIV-1 Infection Requires Multiple Pathways. <i>PLoS Pathogens</i> , 2009, 5, e1000594.	4.7	172
81	Highly complex neutralization determinants on a monophyletic lineage of newly transmitted subtype C HIV-1 Env clones from India. <i>Virology</i> , 2009, 385, 505-520.	2.4	78
82	Conformational Flexibility of Soluble Cellulose Oligomers: Chain Length and Temperature Dependence. <i>Journal of the American Chemical Society</i> , 2009, 131, 14786-14794.	13.7	102
83	The Stability of Cellulose: A Statistical Perspective from a Coarse-Grained Model of Hydrogen-Bond Networks. <i>Biophysical Journal</i> , 2009, 96, 3032-3040.	0.5	109
84	The implications of patterns in HIV diversity for neutralizing antibody induction and susceptibility. <i>Current Opinion in HIV and AIDS</i> , 2009, 4, 408-417.	3.8	50
85	A Dual-Purpose Protein Ligand for Effective Therapy and Sensitive Diagnosis of Anthrax. <i>Protein Journal</i> , 2008, 27, 292-302.	1.6	13
86	The Solvent ¹³ C-Dependent Shift of the Amide I Band of a Fully Solvated Peptide as a Local Probe for the Solvent Composition in the Peptide/Solvent Interface. <i>ChemPhysChem</i> , 2008, 9, 2742-2750.	2.1	15
87	The bioinorganic chemistry and associated immunology of chronic beryllium disease. <i>Chemical Communications</i> , 2008, , 2837.	4.1	57
88	Perturbation of Local Solvent Structure by a Small Dication: A Theoretical Study on Structural, Vibrational, and Reactive Properties of Beryllium Ion in Water. <i>Journal of Physical Chemistry B</i> , 2008, 112, 2958-2963.	2.6	16
89	Unique Mutational Patterns in the Envelope ± 2 Amphipathic Helix and Acquisition of Length in gp120 Hypervariable Domains Are Associated with Resistance to Autologous Neutralization of Subtype C Human Immunodeficiency Virus Type 1. <i>Journal of Virology</i> , 2007, 81, 5658-5668.	3.4	92
90	Clade-Specific Differences between Human Immunodeficiency Virus Type 1 Clades B and C: Diversity and Correlations in C3-V4 Regions of gp120. <i>Journal of Virology</i> , 2007, 81, 4886-4891.	3.4	66

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91	Atomic-Level Description of Amyloid β -Dimer Formation. <i>Journal of the American Chemical Society</i> , 2006, 128, 2158-2159.	13.7	149
92	Consistent Patterns of Change during the Divergence of Human Immunodeficiency Virus Type 1 Envelope from That of the Inoculated Virus in Simian/Human Immunodeficiency Virus-Infected Macaques. <i>Journal of Virology</i> , 2006, 80, 999-1014.	3.4	55
93	Helix-coil transition of alanine peptides in water: Force field dependence on the folded and unfolded structures. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 59, 773-782.	2.6	86
94	Simulations of the pressure and temperature unfolding of an α -helical peptide. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 6765-6770.	7.1	108
95	Atomic Simulations of Protein Folding, Using the Replica Exchange Algorithm. <i>Methods in Enzymology</i> , 2004, 383, 119-149.	1.0	120
96	Nature of structural inhomogeneities on folding a helix and their influence on spectral measurements. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 9229-9234.	7.1	58
97	Peptide folding simulations. <i>Current Opinion in Structural Biology</i> , 2003, 13, 168-174.	5.7	203
98	Validation of an All-Atom Protein Force Field: α From Dipeptides to Larger Peptides. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12555-12557.	2.6	112
99	Folding of a Highly Conserved Diverging Turn Motif from the SH3 Domain. <i>Biophysical Journal</i> , 2003, 84, 1548-1562.	0.5	25
100	Conformational Preferences and Vibrational Frequency Distributions of Short Peptides in Relation to Multidimensional Infrared Spectroscopy. <i>Journal of the American Chemical Society</i> , 2001, 123, 12886-12898.	13.7	106
101	Quantification of the Resilience and Vulnerability of HIV-1 Native Glycan Shield at Atomistic Detail. <i>SSRN Electronic Journal</i> , 0, , .	0.4	4