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List of Publications by Year
in descending order

Version: 2024-02-01

127 papers	9,670 citations	76196 40 h-index	45213 90 g-index
138 all docs	138 docs citations	138 times ranked	10308 citing authors

#	Article	IF	Citations
1	CNN-PepPred: an open-source tool to create convolutional NN models for the discovery of patterns in peptide setsâ€"application to peptideâ€"MHC class II binding prediction. Bioinformatics, 2021, 37, 4567-4568.	1.8	5
2	CuBlock: a cross-platform normalization method for gene-expression microarrays. Bioinformatics, 2021, 37, 2365-2373.	1.8	7
3	The Pseudomonas aeruginosa substrate-binding protein Ttg2D functions as a general glycerophospholipid transporter across the periplasm. Communications Biology, 2021, 4, 448.	2.0	15
4	On the Effect of the Various Assumptions and Approximations used in Molecular Simulations on the Properties of Bioâ€Molecular Systems: Overview and Perspective on Issues. ChemPhysChem, 2021, 22, 264-282.	1.0	12
5	Methods to Develop an in silico Clinical Trial: Computational Head-to-Head Comparison of Lisdexamfetamine and Methylphenidate. Frontiers in Psychiatry, 2021, 12, 741170.	1.3	16
6	Antigen Discovery in Bacterial Panproteomes. Methods in Molecular Biology, 2021, 2183, 43-62.	0.4	6
7	Antibacterial Activity of T22, a Specific Peptidic Ligand of the Tumoral Marker CXCR4. Pharmaceutics, 2021, 13, 1922.	2.0	5
8	Aggregation-prone peptides modulate activity of bovine interferon gamma released from naturally occurring protein nanoparticles. New Biotechnology, 2020, 57, 11-19.	2.4	11
9	Genetic Variants of the DSF Quorum Sensing System in Stenotrophomonas maltophilia Influence Virulence and Resistance Phenotypes Among Genotypically Diverse Clinical Isolates. Frontiers in Microbiology, 2020, 11, 1160.	1.5	22
10	Interaction of camel Lactoferrin derived peptides with DNA: a molecular dynamics study. BMC Genomics, 2020, 21, 60.	1.2	13
11	The phylogenetic landscape and nosocomial spread of the multidrug-resistant opportunist Stenotrophomonas maltophilia. Nature Communications, 2020, 11, 2044.	5.8	76
12	Sulfonamide-based diffusible signal factor analogs interfere with quorum sensing in Stenotrophomonas maltophilia and Burkholderia cepacia. Future Medicinal Chemistry, 2019, 11, 1565-1582.	1.1	15
13	HLA and microtubule-associated protein tau H1 haplotype associations in anti-IgLON5 disease. Neurology: Neuroimmunology and NeuroInflammation, 2019, 6, .	3.1	55
14	Advances in the Computational Identification of Allosteric Sites and Pathways in Proteins. Advances in Experimental Medicine and Biology, 2019, 1163, 141-169.	0.8	14
15	Validierung von molekularen Simulationen: eine Ãœbersicht verschiedener Aspekte. Angewandte Chemie, 2018, 130, 894-915.	1.6	3
16	Validation of Molecular Simulation: An Overview of Issues. Angewandte Chemie - International Edition, 2018, 57, 884-902.	7.2	101
17	Heterogeneous Colistin-Resistance Phenotypes Coexisting in Stenotrophomonas maltophilia Isolates Influence Colistin Susceptibility Testing. Frontiers in Microbiology, 2018, 9, 2871.	1.5	29
18	Quorum Sensing Signaling and Quenching in the Multidrug-Resistant Pathogen Stenotrophomonas maltophilia. Frontiers in Cellular and Infection Microbiology, 2018, 8, 122.	1.8	39

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19	BPSL1626: Reverse and Structural Vaccinology Reveal a Novel Candidate for Vaccine Design Against Burkholderia pseudomallei. Antibodies, 2018, 7, 26.	1.2	11
20	Molecular dynamics simulation study of the effect of glycerol dialkyl glycerol tetraether hydroxylation on membrane thermostability. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 966-974.	1.4	25
21	The fusogenic peptide HA2 impairs selectivity of CXCR4-targeted protein nanoparticles. Chemical Communications, 2017, 53, 4565-4568.	2.2	12
22	A Bowmanâ€“Birk protease inhibitor purified, cloned, sequenced and characterized from the seeds of Maclura pomifera (Raf.) Schneid. Planta, 2017, 245, 343-353.	1.6	7
23	Human Leukocyte Antigen (HLA)-DRB1*15:01 and HLA-DRB5*01:01 Present Complementary Peptide Repertoires. Frontiers in Immunology, 2017, 8, 984.	2.2	25
24	Effect of Oxidative Damage on the Stability and Dimerization of Superoxide Dismutase 1. Biophysical Journal, 2016, 110, 1499-1509.	0.2	53
25	Conformational and functional variants of CD44-targeted protein nanoparticles bio-produced in bacteria. Biofabrication, 2016, 8, 025001.	3.7	15
26	Proteomic analysis of outer membrane proteins and vesicles of a clinical isolate and a collection strain of Stenotrophomonas maltophilia. Journal of Proteomics, 2016, 142, 122-129.	1.2	17
27	Bestimmung von Strukturinformation aus experimentellen Messdaten fÃ¼r BiomolekÃ¼le. Angewandte Chemie, 2016, 128, 16222-16244.	1.6	7
28	Deriving Structural Information from Experimentally Measured Data on Biomolecules. Angewandte Chemie - International Edition, 2016, 55, 15990-16010.	7.2	24
29	A Comparative Analysis of the Peptide Repertoires of HLAâ€“DR Molecules Differentially Associated With Rheumatoid Arthritis. Arthritis and Rheumatology, 2016, 68, 2412-2421.	2.9	10
30	Bottomâ€Up Instructive Quality Control in the Biofabrication of Smart Protein Materials. Advanced Materials, 2015, 27, 7816-7822.	11.1	61
31	Stenotrophomonas maltophilia responds to exogenous AHL signals through the LuxR solo SmoR (Smlt1839). Frontiers in Cellular and Infection Microbiology, 2015, 5, 41.	1.8	38
32	Decoding the genetic and functional diversity of the DSF quorum-sensing system in Stenotrophomonas maltophilia. Frontiers in Microbiology, 2015, 6, 761.	1.5	37
33	Sequence- and Structure-Based Immunoreactive Epitope Discovery for Burkholderia pseudomallei Flagellin. PLoS Neglected Tropical Diseases, 2015, 9, e0003917.	1.3	40
34	Draft Genome Sequence of Stenotrophomonas maltophilia Strain UV74 Reveals Extensive Variability within Its Genomic Group. Genome Announcements, 2015, 3, .	0.8	5
35	PrionW: a server to identify proteins containing glutamine/asparagine rich prion-like domains and their amyloid cores. Nucleic Acids Research, 2015, 43, W331-W337.	6.5	74
36	From crystal structure to inÂsilico epitope discovery in the BurkholderiaÂpseudomallei flagellar hookâ€associated protein FlgK. FEBS Journal, 2015, 282, 1319-1333.	2.2	42

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37	Structure-Based Design of a B Cell Antigen from B. pseudomallei. ACS Chemical Biology, 2015, 10, 803-812.	1.6	12
38	Prediction of Antigenic B and T Cell Epitopes via Energy Decomposition Analysis: Description of the Web-Based Prediction Tool BEPPE. Methods in Molecular Biology, 2015, 1348, 13-22.	0.4	6
39	Two Different rpf Clusters Distributed among a Population of Stenotrophomonas maltophilia Clinical Strains Display Differential Diffusible Signal Factor Production and Virulence Regulation. Journal of Bacteriology, 2014, 196, 2431-2442.	1.0	55
40	Draft Genome Sequence of Stenotrophomonas maltophilia Strain M30, Isolated from a Chronic Pressure Ulcer in an Elderly Patient. Genome Announcements, 2014, 2, .	0.8	4
41	antibacTR: dynamic antibacterial-drug-target ranking integrating comparative genomics, structural analysis and experimental annotation. BMC Genomics, 2014, 15, 36.	1.2	10
42	PARS: a web server for the prediction of Protein Allosteric and Regulatory Sites. Bioinformatics, 2014, 30, 1314-1315.	1.8	117
43	Sheltering DNA in self-organizing, protein-only nano-shells as artificial viruses for gene delivery. Nanomedicine: Nanotechnology, Biology, and Medicine, 2014, 10, 535-541.	1.7	27
44	In Vivo Architectonic Stability of Fully de Novo Designed Protein-Only Nanoparticles. ACS Nano, 2014, 8, 4166-4176.	7.3	89
45	Redefining the PF06864 Pfam Family Based on Burkholderia pseudomallei PilO2Bp S-SAD Crystal Structure. PLoS ONE, 2014, 9, e94981.	1.1	4
46	Exploiting the Burkholderia pseudomallei Acute Phase Antigen BPSL2765 for Structure-Based Epitope Discovery/Design in Structural Vaccinology. Chemistry and Biology, 2013, 20, 1147-1156.	6.2	50
47	Crystal structure of c5321: a protective antigen present in uropathogenic Escherichia coli strains displaying an SLR fold. BMC Structural Biology, 2013, 13, 19.	2.3	17
48	A Structure-Based Strategy for Epitope Discovery in Burkholderia pseudomallei OppA Antigen. Structure, 2013, 21, 167-175.	1.6	49
49	EsiB, a Novel Pathogenic Escherichia coli Secretory Immunoglobulin A-Binding Protein Impairing Neutrophil Activation. MBio, 2013, 4, .	1.8	22
50	Understanding the Molecular Determinants Driving the Immunological Specificity of the Protective Pilus 2a Backbone Protein of Group B Streptococcus. PLoS Computational Biology, 2013, 9, e1003115.	1.5	82
51	Abundance of the Quorum-Sensing Factor Ax21 in Four Strains of Stenotrophomonas maltophilia Correlates with Mortality Rate in a New Zebrafish Model of Infection. PLoS ONE, 2013, 8, e67207.	1.1	33
52	RGD-based cell ligands for cell-targeted drug delivery act as potent trophic factors. Nanomedicine: Nanotechnology, Biology, and Medicine, 2012, 8, 1263-1266.	1.7	16
53	Disulfide Bond Formation and Activation of Escherichia coli Î²-Galactosidase under Oxidizing Conditions. Applied and Environmental Microbiology, 2012, 78, 2376-2385.	1.4	9
54	The Role of Hydration in Protein Stability: Comparison of the Cold and Heat Unfolded States of Yfh1. Journal of Molecular Biology, 2012, 417, 413-424.	2.0	52

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55	Exploiting protein flexibility to predict the location of allosteric sites. BMC Bioinformatics, 2012, 13, 273.	1.2	72
56	Free energy calculations offer insights into the influence of receptor flexibility on ligandâ€“receptor binding affinities. Journal of Computer-Aided Molecular Design, 2011, 25, 709-716.	1.3	10
57	Nanoparticulate architecture of protein-based artificial viruses is supported by proteinâ€“DNA interactions. Nanomedicine, 2011, 6, 1047-1061.	1.7	14
58	Structural and Biochemical Characterization of NarE, an Iron-containing ADP-ribosyltransferase from Neisseria meningitidis. Journal of Biological Chemistry, 2011, 286, 14842-14851.	1.6	16
59	On the Relative Merits of Equilibrium and Nonâ€Equilibrium Simulations for the Estimation of Freeâ€Energy Differences. ChemPhysChem, 2010, 11, 3734-3743.	1.0	9
60	Î±â€Cyclodextrin Hostâ€“Guest Binding: A Computational Study of the Different Driving Forces. Helvetica Chimica Acta, 2010, 93, 2318-2325.	1.0	2
61	Polypeptide folding on a conformationalâ€space network: Dependence of network topology on the structural discretization procedure. Journal of Computational Chemistry, 2010, 31, 1889-1903.	1.5	2
62	Assessing the structural conservation of protein pockets to study functional and allosteric sites: implications for drug discovery. BMC Structural Biology, 2010, 10, 9.	2.3	34
63	Exploiting Antigenic Diversity for Vaccine Design. Journal of Biological Chemistry, 2010, 285, 30126-30138.	1.6	44
64	Enhanced Conformational Sampling in Molecular Dynamics Simulations of Solvated Peptides: Fragment-Based Local Elevation Umbrella Sampling. Journal of Chemical Theory and Computation, 2010, 6, 2598-2621.	2.3	25
65	Protein nanodisk assembling and intracellular trafficking powered by an arginine-rich (R9) peptide. Nanomedicine, 2010, 5, 259-268.	1.7	59
66	Comparing geometric and kinetic cluster algorithms for molecular simulation data. Journal of Chemical Physics, 2010, 132, 074110.	1.2	110
67	Why is a protective antigen protective?. Hum Vaccin, 2009, 5, 872-875.	2.4	5
68	Calcium binding to the purple membrane: A molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2009, 74, 669-681.	1.5	5
69	Molecular Dynamics Simulations of a Reversibly Folding Î²-Heptapeptide in Methanol: Influence of the Treatment of Long-Range Electrostatic Interactions. Journal of Physical Chemistry B, 2009, 113, 3112-3128.	1.2	72
70	Estimating the Temperature Dependence of Peptide Folding Entropies and Free Enthalpies from Total Energies in Molecular Dynamics Simulations. Chemistry - A European Journal, 2008, 14, 5039-5046.	1.7	16
71	The rheumatoid arthritisâ€“associated allele HLAâ€“DR10 (DRB1*1001) shares part of its repertoire with HLAâ€“DR1 (DRB1*0101) and HLAâ€“DR4 (DRB*0401). Arthritis and Rheumatism, 2008, 58, 1630-1639.	6.7	34
72	Thyroglobulin Peptides Associate In Vivo to HLA-DR in Autoimmune Thyroid Glands. Journal of Immunology, 2008, 181, 795-807.	0.4	48

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73	AGGRESCAN: a server for the prediction and evaluation of "hot spots" of aggregation in polypeptides. BMC Bioinformatics, 2007, 8, 65.	1.2	845
74	Configurational entropy elucidates the role of salt-bridge networks in protein thermostability. Protein Science, 2007, 16, 1349-1359.	3.1	99
75	Molecular Dynamics Simulation of Peptide Folding. Theoretical Chemistry Accounts, 2006, 116, 297-306.	0.5	20
76	Biomolecular Modeling: Goals, Problems, Perspectives. Angewandte Chemie - International Edition, 2006, 45, 4064-4092.	7.2	503
77	Molecular-Dynamics Simulations of C- and N-Terminal Peptide Derivatives of GCN4-p1 in Aqueous Solution. Chemistry and Biodiversity, 2005, 2, 1086-1104.	1.0	17
78	Stability of SIV gp32 Fusionâ€Peptide Singleâ€Layer Protofibrils as Monitored by Molecularâ€Dynamics Simulations. Angewandte Chemie - International Edition, 2005, 44, 1065-1067.	7.2	21
79	Stability of SIV gp32 Fusionâ€Peptide Singleâ€Layer Protofibrils as Monitored by Molecularâ€Dynamics Simulations. Angewandte Chemie, 2005, 117, 1089-1091.	1.6	4
80	On the Influence of Charged Side Chains on the Foldingâ€“Unfolding Equilibrium of Î²-Peptides: A Molecular Dynamics Simulation Study. Chemistry - A European Journal, 2005, 11, 7276-7293.	1.7	23
81	A Molecular Dynamics Simulation of the Binding Modes of d-Glutamate and d-Glutamine to Glutamate Racemase. Journal of Chemical Theory and Computation, 2005, 1, 737-749.	2.3	9
82	Engineering the E. coli Î²-galactosidase for the screening of antiviral protease inhibitors. Biochemical and Biophysical Research Communications, 2005, 329, 453-456.	1.0	3
83	Validation of the GROMOS force-field parameter set 45A3 against nuclear magnetic resonance data of hen egg lysozyme. Journal of Biomolecular NMR, 2004, 30, 407-422.	1.6	87
84	Î²-Hairpin folding and stability: molecular dynamics simulations of designed peptides in aqueous solution. Journal of Peptide Science, 2004, 10, 546-565.	0.8	26
85	Modelling of the Complex between a 15-Residue Peptide from mSos2 and the N-Terminal SH3 Domain of Grb2 by Molecular-Dynamics Simulation. Chemistry and Biodiversity, 2004, 1, 505-519.	1.0	3
86	Circular dichroism spectra of Î²-peptides: sensitivity to molecular structure and effects of motional averaging. European Biophysics Journal, 2003, 32, 661-670.	1.2	53
87	A novel approach for designing simple point charge models for liquid water with three interaction sites. Journal of Computational Chemistry, 2003, 24, 1087-1096.	1.5	24
88	Procarboxypeptidase A from the insect pestHelicoverpa armigeraand its derived enzyme. FEBS Journal, 2003, 270, 3026-3035.	0.2	27
89	Molecular dynamics simulations of peptides containing an unnatural amino acid: Dimerization, folding, and protein binding. Proteins: Structure, Function and Bioinformatics, 2003, 54, 116-127.	1.5	17
90	Unfolded state of peptides. Advances in Protein Chemistry, 2002, 62, 341-360.	4.4	40

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91	Aspects of Modeling Biomolecular Structure on the Basis of Spectroscopic or Diffraction Data. Biological Magnetic Resonance, 2002, , 3-35.	0.4	0
92	Can One Derive the Conformational Preference of a Î²-Peptide from Its CD Spectrum?. Journal of the American Chemical Society, 2002, 124, 12972-12978.	6.6	162
93	Derivation of an improved simple point charge model for liquid water: SPC/A and SPC/L. Journal of Chemical Physics, 2002, 116, 9811-9828.	1.2	203
94	Computation of Free Energy. Helvetica Chimica Acta, 2002, 85, 3113-3129.	1.0	99
95	-Peptides with Different Secondary-Structure Preferences: How Different Are Their Conformational Spaces?. Helvetica Chimica Acta, 2002, 85, 3872-3882.	1.0	23
96	Assessing equilibration and convergence in biomolecular simulations. Proteins: Structure, Function and Bioinformatics, 2002, 48, 487-496.	1.5	128
97	Essential dynamics of reversible peptide folding: memory-free conformational dynamics governed by internal hydrogen bonds. Journal of Molecular Biology, 2001, 309, 299-313.	2.0	126
98	Îhe Î²-Peptide Hairpin in Solution:Â Conformational Study of a Î²-Hexapeptide in Methanol by NMR Spectroscopy and MD Simulation. Journal of the American Chemical Society, 2001, 123, 2393-2404.	6.6	193
99	Folding study of an Aib-rich peptide in DMSO by molecular dynamics simulations. Chemical Biology and Drug Design, 2001, 57, 107-118.	1.2	42
100	Entropy calculations on a reversibly folding peptide: Changes in solute free energy cannot explain folding behavior. Proteins: Structure, Function and Bioinformatics, 2001, 43, 45-56.	1.5	97
101	An improved GROMOS96 force field for aliphatic hydrocarbons in the condensed phase. Journal of Computational Chemistry, 2001, 22, 1205-1218.	1.5	814
102	Oligonucleotide Analogues with a Nucleobase-Including Backbone, Part 7, Molecular Dynamics Simulation of a DNA Duplex Containing a 2â€²-Deoxyadenosine 8-(Hydroxymethyl)-Derived Nucleotide. Helvetica Chimica Acta, 2001, 84, 2132-2145.	1.0	10
103	The Key to Solving the Protein-Folding Problem Lies in an Accurate Description of the Denatured State. Angewandte Chemie - International Edition, 2001, 40, 351-355.	7.2	124
104	Reply. Angewandte Chemie - International Edition, 2001, 40, 4616-4618.	7.2	13
105	Calculation of NMR-relaxation parameters for flexible molecules from molecular dynamics simulations. Journal of Biomolecular NMR, 2001, 20, 297-310.	1.6	89
106	A strategy for analysis of (molecular) equilibrium simulations: Configuration space density estimation, clustering, and visualization. Journal of Chemical Physics, 2001, 114, 2079-2089.	1.2	28
107	Entropy calculations on a reversibly folding peptide: Changes in solute free energy cannot explain folding behavior. , 2001, 43, 45.		1
108	The Key to Solving the Protein-Folding Problem Lies in an Accurate Description of the Denatured State. Angewandte Chemie - International Edition, 2001, 40, 351-355.	7.2	3

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109	An improved GROMOS96 force field for aliphatic hydrocarbons in the condensed phase. , 2001, 22, 1205.		13
110	The Key to Solving the Protein-Folding Problem Lies in an Accurate Description of the Denatured State Financial support from the Schweizerischer Nationalfonds (Project no. 21-50929.97) is gratefully acknowledged.. Angewandte Chemie - International Edition, 2001, 40, 351-355.	7.2	20
111	Structure and Conformation ofÎ²-Oligopeptide Derivatives with Simple Proteinogenic Side Chains: Circular Dichroism and Molecular Dynamics Investigations. Helvetica Chimica Acta, 2000, 83, 34-57.	1.0	100
112	Factor Xa: simulation studies with an eye to inhibitor design. Journal of Computer-Aided Molecular Design, 2000, 14, 507-529.	1.3	11
113	A generalized Langevin dynamics approach to model solvent dynamics effects on proteins via a solvent-accessible surface. The carboxypeptidase A inhibitor protein as a model. Theoretical Chemistry Accounts, 2000, 105, 101-109.	0.5	10
114	Peptides of Aminoxy Acids:â€‰ A Molecular Dynamics Simulation Study of Conformational Equilibria under Various Conditions. Journal of the American Chemical Society, 2000, 122, 7461-7466.	6.6	60
115	Peptide folding simulations: no solvent required?. Computer Physics Communications, 1999, 123, 97-102.	3.0	35
116	Folding-unfolding thermodynamics of a ?-heptapeptide from equilibrium simulations. , 1999, 34, 269-280.		370
117	The effect of motional averaging on the calculation of NMR-derived structural properties. , 1999, 36, 542-555.		103
118	Peptide Folding: When Simulation Meets Experiment. Angewandte Chemie - International Edition, 1999, 38, 236-240.	7.2	1,611
119	Validation of molecular simulation by comparison with experiment: Rotational reorientation of tryptophan in water. Journal of Chemical Physics, 1999, 110, 3049-3055.	1.2	38
120	Peptide Folding: When Simulation Meets Experiment. , 1999, 38, 236.		57
121	Parametrization of aliphatic CHn united atoms of GROMOS96 force field. , 1998, 19, 535-547.		370
122	Reversible peptide folding in solution by molecular dynamics simulation 1 1Edited by R. Huber. Journal of Molecular Biology, 1998, 280, 925-932.	2.0	379
123	Studying the Stability of a Helical Î²â€Heptapeptide by Molecular Dynamics Simulations. Chemistry - A European Journal, 1997, 3, 1410-1417.	1.7	120
124	Free Energies of Transfer of Trp Analogs from Chloroform to Water:Â Comparison of Theory and Experiment and the Importance of Adequate Treatment of Electrostatic and Internal Interactions. Journal of the American Chemical Society, 1996, 118, 6285-6294.	6.6	52
125	On the sensitivity of MD trajectories to changes in water-protein interaction parameters: The potato carboxypeptidase inhibitor in water as a test case for the GROMOS force field. , 1996, 25, 89-103.		37
126	On the Entropic and Hydrophobic Properties Involved in the Inhibitory Mechanism of Carboxypeptidase A by its Natural Inhibitor from Potato. Journal of Molecular Modeling, 1995, 1, 54-67.	0.8	3

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127	Structure and atomic fluctuation patterns of potato carboxypeptidase a inhibitor protein. European Biophysics Journal, 1995, 24, 1-11.	1.2	7