Nicholas M Glykos

List of Publications by Year
in descending order

53	1,289	471509 17	361022 35
papers	citations	h-index	g-index

55	55	55	1904
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Software news and updates carma: A molecular dynamics analysis program. Journal of Computational Chemistry, 2006, 27, 1765-1768.	3.3	385
2	Grcarma: A fully automated taskâ€oriented interface for the analysis of molecular dynamics trajectories. Journal of Computational Chemistry, 2013, 34, 2310-2312.	3.3	108
3	Protein Flexibility and Enzymatic Catalysis. Advances in Protein Chemistry and Structural Biology, 2012, 87, 181-218.	2.3	88
4	Determination of protein oligomerization state: Two approaches based on glutaraldehyde crosslinking. Analytical Biochemistry, 2008, 373, 404-406.	2.4	67
5	Structure of HrcQB-C, a conserved component of the bacterial type III secretion systems. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 70-75.	7.1	62
6	Protein plasticity to the extreme: changing the topology of a 4-Î±-helical bundle with a single amino acid substitution. Structure, 1999, 7, 597-603.	3.3	54
7	Three Force Fields' Views of the 310 Helix. Biophysical Journal, 2011, 101, 1766-1771.	0.5	46
8	Reconstruction of DNA sequences using genetic algorithms and cellular automata: Towards mutation prediction?. BioSystems, 2008, 92, 61-68.	2.0	42
9	The structure of AhrC, the arginine repressor/activator protein fromBacillus subtilis. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 421-430.	2.5	37
10	Crystal structure of the BcZBP, a zinc-binding protein from Bacillus cereus. FEBS Journal, 2007, 274, 3044-3054.	4.7	28
11	A stochastic approach to molecular replacement. Acta Crystallographica Section D: Biological Crystallography, 2000, 56, 169-174.	2.5	24
12	Molecular simulation of peptides coming of age: Accurate prediction of folding, dynamics and structures. Archives of Biochemistry and Biophysics, 2019, 664, 76-88.	3.0	23
13	Using J-Coupling Constants for Force Field Validation: Application to Hepta-alanine. Journal of Physical Chemistry B, 2011, 115, 15221-15227.	2.6	22
14	On the Application of Good-Turing Statistics to Quantify Convergence of Biomolecular Simulations. Journal of Chemical Information and Modeling, 2014, 54, 209-217.	5.4	21
15	Folding Molecular Dynamics Simulations Accurately Predict the Effect of Mutations on the Stability and Structure of a Vammin-Derived Peptide. Journal of Physical Chemistry B, 2014, 118, 10076-10084.	2.6	21
16	Unusual Î±-Carbon Hydroxylation of Proline Promotes Active-Site Maturation. Journal of the American Chemical Society, 2017, 139, 5330-5337.	13.7	20
17	Structure determination through homology modelling and torsion-angle simulated annealing: application to a polysaccharide deacetylase fromBacillus cereus. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 276-283.	2.5	19
18	Loopless Rop:Â Structure and Dynamics of an Engineered Homotetrameric Variant of the Repressor of Primer Protein. Biochemistry, 2006, 45, 10905-10919.	2.5	17

#	Article	IF	Citations
19	Sensitivity of Folding Molecular Dynamics Simulations to Even Minor Force Field Changes. Journal of Chemical Information and Modeling, 2016, 56, 2035-2041.	5.4	14
20	Order through Disorder: Hyper-Mobile C-Terminal Residues Stabilize the Folded State of a Helical Peptide. A Molecular Dynamics Study. PLoS ONE, 2010, 5, e15290.	2.5	14
21	Multidimensional molecular replacement. Acta Crystallographica Section D: Biological Crystallography, 2001, 57, 1462-1473.	2.5	13
22	Structure determination of a small protein through a 23-dimensional molecular-replacement search. Acta Crystallographica Section D: Biological Crystallography, 2003, 59, 709-718.	2.5	13
23	Structural polymorphism of a marginally stable 4-Î±-helical bundle. Images of a trapped molten globule?. Proteins: Structure, Function and Bioinformatics, 2004, 56, 420-425.	2.6	13
24	On the Foldability of Tryptophan-Containing Tetra- and Pentapeptides: An Exhaustive Molecular Dynamics Study. Journal of Physical Chemistry B, 2013, 117, 5522-5532.	2.6	13
25	Characterizing a partially ordered miniprotein through folding molecular dynamics simulations: Comparison with the experimental data. Protein Science, 2016, 25, 587-596.	7.6	11
26	On the quaternary association of the type III secretion system HrcQB-C protein: Experimental evidence differentiates among the various oligomerization models. Journal of Structural Biology, 2009, 166, 214-225.	2.8	10
27	As good as it gets? Folding molecular dynamics simulations of the LytA choline-binding peptide result to an exceptionally accurate model of the peptide structure. Journal of Molecular Graphics and Modelling, 2013, 41, 68-71.	2.4	10
28	Catalytic activity regulation through post-translational modification: the expanding universe of protein diversity. Advances in Protein Chemistry and Structural Biology, 2020, 122, 97-125.	2.3	10
29	Molecular Dynamics Simulations of BcZBP, A Deacetylase from Bacillus cereus: Active Site Loops Determine Substrate Accessibility and Specificity. Journal of Chemical Theory and Computation, 2009, 5, 3299-3311.	5.3	9
30	Folding Simulations of a Nuclear Receptor Box-Containing Peptide Demonstrate the Structural Persistence of the LxxLL Motif Even in the Absence of Its Cognate Receptor. Journal of Physical Chemistry B, 2018, 122, 106-116.	2.6	9
31	On the application of molecular-dynamics simulations to validate thermal parameters and to optimize TLS-group selection for macromolecular refinement. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 705-713.	2.5	8
32	Side-chain conformations in 4-Î±-helical bundles. Protein Engineering, Design and Selection, 2001, 14, 321-328.	2.1	7
33	A Fast and Inexpensive Procedure for Drying Polyacrylamide Gels. Analytical Biochemistry, 2000, 287, 185-186.	2.4	6
34	GraphEnt: a maximum-entropy program with graphics capabilities. Journal of Applied Crystallography, 2000, 33, 982-985.	4.5	6
35	On the distribution of the bulk-solvent correction parameters. Acta Crystallographica Section D: Biological Crystallography, 2000, 56, 1070-1072.	2.5	5
36	Pinda: A Web service for detection and analysis of intraspecies gene duplication events. Computer Methods and Programs in Biomedicine, 2013, 111, 711-714.	4.7	5

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37	Meaningful refinement of polyalanine models using rigid-body simulated annealing: application to the structure determination of the A31P Rop mutant. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 1301-1308.	2.5	4
38	Molecular replacement with multiple different models. Journal of Applied Crystallography, 2004, 37, 159-161.	4.5	4
39	Folding Molecular Dynamics Simulation of a gp41-Derived Peptide Reconcile Divergent Structure Determinations. ACS Omega, 2018, 3, 14746-14754.	3.5	4
40	Ionic strength reducers: an efficient approach to protein purification and crystallization. Application to two Rop variants. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 1334-1337.	2.5	3
41	The balance between sideâ€chain and backboneâ€driven association in folding of the Î±â€helical influenza A transmembrane peptide. Journal of Computational Chemistry, 2020, 41, 2177-2188.	3.3	3
42	Pepinsky's Machine: an interactive graphics-based Fourier synthesis program with applications in teaching and research. Journal of Applied Crystallography, 1999, 32, 821-823.	4.5	2
43	Qs v.1.3: a parallel version of Queen of Spades. Journal of Applied Crystallography, 2005, 38, 574-575.	4.5	2
44	On the application of structure-specific bulk-solvent models. Acta Crystallographica Section D: Biological Crystallography, 2011, 67, 739-741.	2.5	2
45	A molecular dynamics simulation study on the propensity of Asn-Gly-containing heptapeptides towards Î²-turn structures: Comparison with ab initio quantum mechanical calculations. PLoS ONE, 2020, 15, e0243429.	2.5	2
46	Low-Resolution Structural Characterization of the Arginine Repressor/Activator fromBacillus subtilis: a Combined X-ray Crystallographic and Electron Microscopical Approach. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 215-225.	2.5	1
47	Crystallization of type I chloramphenicol acetyltransferase: an approach based on the concept of ionic strength reducers. Acta Crystallographica Section D: Biological Crystallography, 2000, 56, 101-103.	2.5	1
48	The 11th Misconception?. CBE Life Sciences Education, 2011, 10, 1-2.	2.3	1
49	Crystallization and diffraction to ultrahigh resolution (0.8â€…Ã…) of a designed variant of the Rop protein. Acta Crystallographica Section D: Biological Crystallography, 2000, 56, 1015-1016.	2.5	0
50	On the presence of shortâ€range periodicities in protein structures that are not related to established secondary structure elements. Proteins: Structure, Function and Bioinformatics, 2019, 87, 966-978.	2.6	0
51	Stochastic molecular replacement. NATO Science Series Series II, Mathematics, Physics and Chemistry, 2007, , 79-90.	0.1	0
52	Low-Resolution Structural Characterization of the Arginine Repressor/Activator from Bacillus subtilis: a Combined X-ray Crystallographic and Electron Microscopical Approach. Erratum. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 707-707.	2.5	0
53	Folding molecular dynamics simulation of Tâ€peptide, a <scp>HIV</scp> viral entry inhibitor: Structure, dynamics, and comparison with the experimental data. Journal of Computational Chemistry, 2022, 43, 942-952.	3.3	0