

Nicholas M Glykos

List of Publications by Year in descending order

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53
papers

1,289
citations

471509

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361022

35
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55
docs citations

55
times ranked

1904
citing authors

#	ARTICLE	IF	CITATIONS
1	Folding molecular dynamics simulation of Tâ€peptide, a <sc>HIV</sc> viral entry inhibitor: Structure, dynamics, and comparison with the experimental data. <i>Journal of Computational Chemistry</i> , 2022, 43, 942-952.	3.3	0
2	The balance between sideâ€chain and backboneâ€driven association in folding of the Î±â€helical influenza A transmembrane peptide. <i>Journal of Computational Chemistry</i> , 2020, 41, 2177-2188.	3.3	3
3	Catalytic activity regulation through post-translational modification: the expanding universe of protein diversity. <i>Advances in Protein Chemistry and Structural Biology</i> , 2020, 122, 97-125.	2.3	10
4	A molecular dynamics simulation study on the propensity of Asn-Gly-containing heptapeptides towards Î²-turn structures: Comparison with ab initio quantum mechanical calculations. <i>PLoS ONE</i> , 2020, 15, e0243429.	2.5	2
5	Molecular simulation of peptides coming of age: Accurate prediction of folding, dynamics and structures. <i>Archives of Biochemistry and Biophysics</i> , 2019, 664, 76-88.	3.0	23
6	On the presence of shortâ€range periodicities in protein structures that are not related to established secondary structure elements. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 966-978.	2.6	0
7	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. <i>Journal of Physical Chemistry B</i> , 2018, 122, 106-116.	2.6	9
8	Folding Molecular Dynamics Simulation of a gp41-Derived Peptide Reconcile Divergent Structure Determinations. <i>ACS Omega</i> , 2018, 3, 14746-14754.	3.5	4
9	Unusual Î±-Carbon Hydroxylation of Proline Promotes Active-Site Maturation. <i>Journal of the American Chemical Society</i> , 2017, 139, 5330-5337.	13.7	20
10	Sensitivity of Folding Molecular Dynamics Simulations to Even Minor Force Field Changes. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 2035-2041.	5.4	14
11	Characterizing a partially ordered miniprotein through folding molecular dynamics simulations: Comparison with the experimental data. <i>Protein Science</i> , 2016, 25, 587-596.	7.6	11
12	On the Application of Good-Turing Statistics to Quantify Convergence of Biomolecular Simulations. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 209-217.	5.4	21
13	Folding Molecular Dynamics Simulations Accurately Predict the Effect of Mutations on the Stability and Structure of a Vammin-Derived Peptide. <i>Journal of Physical Chemistry B</i> , 2014, 118, 10076-10084.	2.6	21
14	Grcarma: A fully automated taskâ€oriented interface for the analysis of molecular dynamics trajectories. <i>Journal of Computational Chemistry</i> , 2013, 34, 2310-2312.	3.3	108
15	Pinda: A Web service for detection and analysis of intraspecies gene duplication events. <i>Computer Methods and Programs in Biomedicine</i> , 2013, 111, 711-714.	4.7	5
16	On the Foldability of Tryptophan-Containing Tetra- and Pentapeptides: An Exhaustive Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5522-5532.	2.6	13
17	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. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 41, 68-71.	2.4	10
18	Structure determination through homology modelling and torsion-angle simulated annealing: application to a polysaccharide deacetylase from <i>Bacillus cereus</i>. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 276-283.	2.5	19

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19	Protein Flexibility and Enzymatic Catalysis. <i>Advances in Protein Chemistry and Structural Biology</i> , 2012, 87, 181-218.	2.3	88
20	Using $\langle i \rangle$ -Coupling Constants for Force Field Validation: Application to Hepta-alanine. <i>Journal of Physical Chemistry B</i> , 2011, 115, 15221-15227.	2.6	22
21	Three Force Fields' Views of the 310 Helix. <i>Biophysical Journal</i> , 2011, 101, 1766-1771.	0.5	46
22	On the application of structure-specific bulk-solvent models. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011, 67, 739-741.	2.5	2
23	The 11th Misconception?. <i>CBE Life Sciences Education</i> , 2011, 10, 1-2.	2.3	1
24	Order through Disorder: Hyper-Mobile C-Terminal Residues Stabilize the Folded State of a Helical Peptide. A Molecular Dynamics Study. <i>PLoS ONE</i> , 2010, 5, e15290.	2.5	14
25	Molecular Dynamics Simulations of BcZBP, A Deacetylase from <i>Bacillus cereus</i> : Active Site Loops Determine Substrate Accessibility and Specificity. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3299-3311.	5.3	9
26	On the quaternary association of the type III secretion system HrcQB-C protein: Experimental evidence differentiates among the various oligomerization models. <i>Journal of Structural Biology</i> , 2009, 166, 214-225.	2.8	10
27	Reconstruction of DNA sequences using genetic algorithms and cellular automata: Towards mutation prediction?. <i>BioSystems</i> , 2008, 92, 61-68.	2.0	42
28	Determination of protein oligomerization state: Two approaches based on glutaraldehyde crosslinking. <i>Analytical Biochemistry</i> , 2008, 373, 404-406.	2.4	67
29	On the application of molecular-dynamics simulations to validate thermal parameters and to optimize TLS-group selection for macromolecular refinement. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2007, 63, 705-713.	2.5	8
30	Crystal structure of the BcZBP, a zinc-binding protein from <i>Bacillus cereus</i> . <i>FEBS Journal</i> , 2007, 274, 3044-3054.	4.7	28
31	Stochastic molecular replacement. <i>NATO Science Series Series II, Mathematics, Physics and Chemistry</i> , 2007, , 79-90.	0.1	0
32	Loopless Rop: Structure and Dynamics of an Engineered Homotetrameric Variant of the Repressor of Primer Protein. <i>Biochemistry</i> , 2006, 45, 10905-10919.	2.5	17
33	Software news and updates carma: A molecular dynamics analysis program. <i>Journal of Computational Chemistry</i> , 2006, 27, 1765-1768.	3.3	385
34	Qs v.1.3: a parallel version of Queen of Spades. <i>Journal of Applied Crystallography</i> , 2005, 38, 574-575.	4.5	2
35	Structure of HrcQB-C, a conserved component of the bacterial type III secretion systems. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 70-75.	7.1	62
36	Structural polymorphism of a marginally stable 4-helical bundle. Images of a trapped molten globule?. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 56, 420-425.	2.6	13

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37	Ionic strength reducers: an efficient approach to protein purification and crystallization. Application to two Rop variants. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 1334-1337.	2.5	3
38	Molecular replacement with multiple different models. <i>Journal of Applied Crystallography</i> , 2004, 37, 159-161.	4.5	4
39	Structure determination of a small protein through a 23-dimensional molecular-replacement search. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2003, 59, 709-718.	2.5	13
40	The structure of AhrC, the arginine repressor/activator protein from <i>Bacillus subtilis</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 421-430.	2.5	37
41	Multidimensional molecular replacement. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2001, 57, 1462-1473.	2.5	13
42	Side-chain conformations in 4- $\hat{1}$ -helical bundles. <i>Protein Engineering, Design and Selection</i> , 2001, 14, 321-328.	2.1	7
43	A Fast and Inexpensive Procedure for Drying Polyacrylamide Gels. <i>Analytical Biochemistry</i> , 2000, 287, 185-186.	2.4	6
44	GraphEnt: a maximum-entropy program with graphics capabilities. <i>Journal of Applied Crystallography</i> , 2000, 33, 982-985.	4.5	6
45	Crystallization and diffraction to ultrahigh resolution (0.8 \hat{A} ...) of a designed variant of the Rop protein. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2000, 56, 1015-1016.	2.5	0
46	On the distribution of the bulk-solvent correction parameters. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2000, 56, 1070-1072.	2.5	5
47	Crystallization of type I chloramphenicol acetyltransferase: an approach based on the concept of ionic strength reducers. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2000, 56, 101-103.	2.5	1
48	A stochastic approach to molecular replacement. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2000, 56, 169-174.	2.5	24
49	Pepinsky's Machine: an interactive graphics-based Fourier synthesis program with applications in teaching and research. <i>Journal of Applied Crystallography</i> , 1999, 32, 821-823.	4.5	2
50	Meaningful refinement of polyalanine models using rigid-body simulated annealing: application to the structure determination of the A31P Rop mutant. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 1301-1308.	2.5	4
51	Protein plasticity to the extreme: changing the topology of a 4- $\hat{1}$ -helical bundle with a single amino acid substitution. <i>Structure</i> , 1999, 7, 597-603.	3.3	54
52	Low-Resolution Structural Characterization of the Arginine Repressor/Activator from <i>Bacillus subtilis</i> : a Combined X-ray Crystallographic and Electron Microscopical Approach. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1998, 54, 215-225.	2.5	1
53	Low-Resolution Structural Characterization of the Arginine Repressor/Activator from <i>Bacillus subtilis</i> : a Combined X-ray Crystallographic and Electron Microscopical Approach. Erratum. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1998, 54, 707-707.	2.5	0