

Jens Erik Nielsen

List of Publications by Year in descending order

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35
papers

3,126
citations

394421

19
h-index

377865

34
g-index

35
all docs

35
docs citations

35
times ranked

4779
citing authors

#	ARTICLE	IF	CITATIONS
1	Predicting Changes in the Stability of Proteins and Protein Complexes: A Study of More Than 1000 Mutations. <i>Journal of Molecular Biology</i> , 2002, 320, 369-387.	4.2	1,609
2	Protein engineering of bacterial α -amylases. <i>BBA - Proteins and Proteomics</i> , 2000, 1543, 253-274.	2.1	235
3	Progress in the prediction of pK_a values in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 3260-3275.	2.6	229
4	Calculating pK_a values in enzyme active sites. <i>Protein Science</i> , 2003, 12, 1894-1901.	7.6	147
5	On the evaluation and optimization of protein X-ray structures for pK_a calculations. <i>Protein Science</i> , 2003, 12, 313-326.	7.6	108
6	The determinants of α -amylase pH -activity profiles. <i>Protein Engineering, Design and Selection</i> , 2001, 14, 505-512.	2.1	92
7	Remeasuring HEWL pK_a values by NMR spectroscopy: Methods, analysis, accuracy, and implications for theoretical pK_a calculations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 685-702.	2.6	89
8	Protein Dielectric Constants Determined from NMR Chemical Shift Perturbations. <i>Journal of the American Chemical Society</i> , 2013, 135, 16968-16976.	13.7	82
9	Electrostatics in proteins and protein-ligand complexes. <i>Future Medicinal Chemistry</i> , 2010, 2, 647-666.	2.3	75
10	Redesigning protein pK_a values. <i>Protein Science</i> , 2006, 16, 239-249.	7.6	59
11	The ionization of a buried glutamic acid is thermodynamically linked to the stability of <i>Leishmania mexicana</i> triose phosphate isomerase. <i>FEBS Journal</i> , 2000, 267, 2516-2524.	0.2	49
12	Structural Artifacts in Protein-Ligand X-ray Structures: Implications for the Development of Docking Scoring Functions. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 5673-5684.	6.4	49
13	Analysing the pH-dependent properties of proteins using pK_a calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 25, 691-699.	2.4	38
14	Titration_DB: Storage and analysis of NMR-monitored protein pH titration curves. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 843-857.	2.6	37
15	pK_D : re-designing protein pK_a values. <i>Nucleic Acids Research</i> , 2006, 34, W48-W51.	14.5	33
16	Determination of Electrostatic Interaction Energies and Protonation State Populations in Enzyme Active Sites. <i>Journal of Molecular Biology</i> , 2008, 376, 269-287.	4.2	28
17	Chapter 9 Analyzing Enzymatic pH Activity Profiles and Protein Titration Curves Using Structure-Based pK_a Calculations and Titration Curve Fitting. <i>Methods in Enzymology</i> , 2009, 454, 233-258.	1.0	20
18	Improving the analysis of NMR spectra tracking pH-induced conformational changes: Removing artefacts of the electric field on the NMR chemical shift. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 971-984.	2.6	20

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19	Integrated prediction of the effect of mutations on multiple protein characteristics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 165-178.	2.6	19
20	On the development of protein pK_a calculation algorithms. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 3287-3298.	2.6	19
21	Coupled effect of salt and pH on proteins probed with NMR spectroscopy. <i>Chemical Physics Letters</i> , 2013, 579, 114-121.	2.6	13
22	Structure and Dynamics of a Promiscuous Xanthan Lyase from <i>Paenibacillus nanensis</i> and the Design of Variants with Increased Stability and Activity. <i>Cell Chemical Biology</i> , 2019, 26, 191-202.e6.	5.2	13
23	Highly Perturbed pK_a Values in the Unfolded State of Hen Egg White Lysozyme. <i>Biophysical Journal</i> , 2012, 102, 1636-1645.	0.5	9
24	Designed Human Serum Hyaluronidase 1 Variant, HYAL1 ^H L, Exhibits Activity up to pH 5.9. <i>Journal of Biological Chemistry</i> , 2009, 284, 19173-19177.	3.4	8
25	Structure of a GH51 α -arabinofuranosidase from <i>Meripilus giganteus</i> : conserved substrate recognition from bacteria to fungi. <i>Acta Crystallographica Section D: Structural Biology</i> , 2020, 76, 1124-1133.	2.3	8
26	Predicting the open conformations of protein kinases using molecular dynamics simulations. <i>Biopolymers</i> , 2012, 97, 65-72.	2.4	7
27	Investigation of Ionization Pattern of the Adjacent Acidic Residues in the DXDXE Motif of GH-18 Chitinases Using Theoretical pK_a Calculations. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 572-583.	5.4	7
28	Toward Fast Determination of Protein Stability Maps: Experimental and Theoretical Analysis of Mutants of a <i>Nocardioopsis prasina</i> Serine Protease. <i>Biochemistry</i> , 2012, 51, 5339-5347.	2.5	6
29	Capturing, sharing and analysing biophysical data from protein engineering and protein characterization studies. <i>Nucleic Acids Research</i> , 2010, 38, e186-e186.	14.5	5
30	Analyzing Protein NMR pH-Titration Curves. <i>Annual Reports in Computational Chemistry</i> , 2008, 4, 89-106.	1.7	4
31	Calculating pK_a values in the cAMP-dependent protein kinase: The effect of conformational change and ligand binding. <i>Protein Science</i> , 2010, 19, 2485-2497.	7.6	4
32	Constructing and Evaluating Predictive Models for Protein Biophysical Characteristics. <i>Annual Reports in Computational Chemistry</i> , 2011, , 101-124.	1.7	2
33	DataPipeline: Automated importing and fitting of large amounts of biophysical data. <i>Journal of Computational Chemistry</i> , 2012, 33, 2357-2362.	3.3	2
34	A collaborative environment for developing and validating predictive tools for protein biophysical characteristics. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 387-396.	2.9	1
35	Rational Redesign of Enzymes. , 2003, , .		0