## Jens Erik Nielsen

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Structure of a GH51 α- <scp>L</scp> -arabinofuranosidase from <i>Meripilus giganteus</i> : conserved substrate recognition from bacteria to fungi. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1124-1133.	2.3	8
2	Structure and Dynamics of a Promiscuous Xanthan Lyase from Paenibacillus nanensis and the Design of Variants with Increased Stability and Activity. Cell Chemical Biology, 2019, 26, 191-202.e6.	5.2	13
3	Investigation of Ionization Pattern of the Adjacent Acidic Residues in the DXDXE Motif of GH-18 Chitinases Using Theoretical p <i>K</i> <sub>a</sub> Calculations. Journal of Chemical Information and Modeling, 2017, 57, 572-583.	5.4	7
4	Coupled effect of salt and pH on proteins probed with NMR spectroscopy. Chemical Physics Letters, 2013, 579, 114-121.	2.6	13
5	Protein Dielectric Constants Determined from NMR Chemical Shift Perturbations. Journal of the American Chemical Society, 2013, 135, 16968-16976.	13.7	82
6	Highly Perturbed pKa Values in the Unfolded State of Hen Egg White Lysozyme. Biophysical Journal, 2012, 102, 1636-1645.	0.5	9
7	DataPipeline: Automated importing and fitting of large amounts of biophysical data. Journal of Computational Chemistry, 2012, 33, 2357-2362.	3.3	2
8	Toward Fast Determination of Protein Stability Maps: Experimental and Theoretical Analysis of Mutants of a <i>Nocardiopsis prasina</i> Serine Protease. Biochemistry, 2012, 51, 5339-5347.	2.5	6
9	A collaborative environment for developing and validating predictive tools for protein biophysical characteristics. Journal of Computer-Aided Molecular Design, 2012, 26, 387-396.	2.9	1
10	Predicting the open conformations of protein kinases using molecular dynamics simulations. Biopolymers, 2012, 97, 65-72.	2.4	7
11	Constructing and Evaluating Predictive Models for Protein Biophysical Characteristics. Annual Reports in Computational Chemistry, 2011, , 101-124.	1.7	2
12	Integrated prediction of the effect of mutations on multiple protein characteristics. Proteins: Structure, Function and Bioinformatics, 2011, 79, 165-178.	2.6	19
13	Remeasuring HEWL pK <sub>a</sub> values by NMR spectroscopy: Methods, analysis, accuracy, and implications for theoretical pK <sub>a</sub> calculations. Proteins: Structure, Function and Bioinformatics, 2011, 79, 685-702.	2.6	89
14	On the development of protein p <i>K</i> <sub>a</sub> calculation algorithms. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3287-3298.	2.6	19
15	Progress in the prediction of p <i>K</i> <sub>a</sub> values in proteins. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3260-3275.	2.6	229
16	Calculating p <i>K</i> <sub>a</sub> values in the cAMPâ€dependent protein kinase: The effect of conformational change and ligand binding. Protein Science, 2010, 19, 2485-2497.	7.6	4
17	Titration_DB: Storage and analysis of NMRâ€monitored protein pH titration curves. Proteins: Structure, Function and Bioinformatics, 2010, 78, 843-857.	2.6	37
18	Improving the analysis of NMR spectra tracking pHâ€induced conformational changes: Removing artefacts of the electric field on the NMR chemical shift. Proteins: Structure, Function and Bioinformatics, 2010, 78, 971-984.	2.6	20

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19	Capturing, sharing and analysing biophysical data from protein engineering and protein characterization studies. Nucleic Acids Research, 2010, 38, e186-e186.	14.5	5
20	Electrostatics in proteins and protein–ligand complexes. Future Medicinal Chemistry, 2010, 2, 647-666.	2.3	75
21	Designed Human Serum Hyaluronidase 1 Variant, HYAL1ΔL, Exhibits Activity up to pH 5.9. Journal of Biological Chemistry, 2009, 284, 19173-19177.	3.4	8
22	Structural Artifacts in Proteinâ^'Ligand X-ray Structures: Implications for the Development of Docking Scoring Functions. Journal of Medicinal Chemistry, 2009, 52, 5673-5684.	6.4	49
23	Chapter 9 Analyzing Enzymatic pH Activity Profiles and Protein Titration Curves Using Structure-Based pKa Calculations and Titration Curve Fitting. Methods in Enzymology, 2009, 454, 233-258.	1.0	20
24	Analyzing Protein NMR pH-Titration Curves. Annual Reports in Computational Chemistry, 2008, 4, 89-106.	1.7	4
25	Determination of Electrostatic Interaction Energies and Protonation State Populations in Enzyme Active Sites. Journal of Molecular Biology, 2008, 376, 269-287.	4.2	28
26	Analysing the pH-dependent properties of proteins using pKa calculations. Journal of Molecular Graphics and Modelling, 2007, 25, 691-699.	2.4	38
27	Redesigning protein pKa values. Protein Science, 2006, 16, 239-249.	7.6	59
28	pKD: re-designing protein pKa values. Nucleic Acids Research, 2006, 34, W48-W51.	14.5	33
29	Calculating pKa values in enzyme active sites. Protein Science, 2003, 12, 1894-1901.	7.6	147
30	On the evaluation and optimization of protein X-ray structures for pKa calculations. Protein Science, 2003, 12, 313-326.	7.6	108
31	Rational Redesign of Enzymes. , 2003, , .		0
32	Predicting Changes in the Stability of Proteins and Protein Complexes: A Study of More Than 1000 Mutations. Journal of Molecular Biology, 2002, 320, 369-387.	4.2	1,609
33	The determinants of α-amylase pH–activity profiles. Protein Engineering, Design and Selection, 2001, 14, 505-512.	2.1	92
34	The ionization of a buried glutamic acid is thermodynamically linked to the stability of Leishmania mexicana triose phosphate isomerase. FEBS Journal, 2000, 267, 2516-2524.	0.2	49
35	Protein engineering of bacterial α-amylases. BBA - Proteins and Proteomics, 2000, 1543, 253-274.	2.1	235