

Water penetration and escape in proteins

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Citation Report

#	ARTICLE	IF	CITATIONS
1	High Apparent Dielectric Constants in the Interior of a Protein Reflect Water Penetration. <i>Biophysical Journal</i> , 2000, 79, 1610-1620.	0.2	295
2	Functional Dynamics of the Hydrophobic Cleft in the N-Domain of Calmodulin. <i>Biophysical Journal</i> , 2001, 80, 2082-2092.	0.2	78
3	Femtosecond Dynamics of Intracellular Water Probed with Nonlinear Optical Kerr Effect Microspectroscopy. <i>Biophysical Journal</i> , 2001, 80, 3019-3024.	0.2	59
4	Gaussian fluctuations and linear response in an electron transfer protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 6544-6549.	3.3	92
5	Protein folding mediated by solvation: Water expulsion and formation of the hydrophobic core occur after the structural collapse. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 685-690.	3.3	461
6	Molecular Dynamics Study of <i>Desulfovibrio africanus</i> Cytochrome c3 in Oxidized and Reduced Forms. <i>Biophysical Journal</i> , 2002, 83, 3049-3065.	0.2	12
7	Properties of Water Molecules in the Active Site Gorge of Acetylcholinesterase from Computer Simulation. <i>Biophysical Journal</i> , 2002, 82, 2671-2682.	0.2	48
8	Experimental pKa Values of Buried Residues: Analysis with Continuum Methods and Role of Water Penetration. <i>Biophysical Journal</i> , 2002, 82, 3289-3304.	0.2	193
9	Posttransition State Desolvation of the Hydrophobic Core of the src-SH3 Protein Domain. <i>Biophysical Journal</i> , 2003, 85, 61-69.	0.2	40
10	A discrete water exit pathway in the membrane protein cytochrome c oxidase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003, 100, 15539-15542.	3.3	69
11	Molecular structure and hydrophobic solvation thermodynamics at an octane-water interface. <i>Journal of Chemical Physics</i> , 2003, 119, 9199-9206.	1.2	77
12	Water and proteins: A love-hate relationship. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 3325-3326.	3.3	168
13	Water clusters in nonpolar cavities. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 17002-17005.	3.3	222
14	Incorporation of the fluorescent amino acid 7-azatryptophan into the core domain 1-47 of hirudin as a probe of hirudin folding and thrombin recognition. <i>Protein Science</i> , 2004, 13, 1489-1502.	3.1	50
15	Two different proteins that compete for binding to thrombin have opposite kinetic and thermodynamic profiles. <i>Protein Science</i> , 2004, 13, 166-176.	3.1	45
16	Hydration of Enzyme in Nonaqueous Media Is Consistent with Solvent Dependence of Its Activity. <i>Biophysical Journal</i> , 2004, 87, 812-821.	0.2	219
17	Dynamic Water Networks in Cytochrome c Oxidase from <i>Paracoccus denitrificans</i> Investigated by Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2004, 86, 1873-1889.	0.2	93
18	Water Molecules and Hydrogen-Bonded Networks in Bacteriorhodopsin-Molecular Dynamics Simulations of the Ground State and the M-Intermediate. <i>Biophysical Journal</i> , 2005, 88, 3252-3261.	0.2	51

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19	Local Compressibilities of Proteins: Comparison of Optical Experiments and Simulations for Horse Heart Cytochrome-c. <i>Biophysical Journal</i> , 2005, 89, 64-75.	0.2	27
20	Anesthetic Interaction with Ketosteroid Isomerase: Insights from Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2005, 89, 2350-2356.	0.2	18
21	Role of Protein Cavities on Unfolding Volume Change and on Internal Dynamics under Pressure. <i>Biophysical Journal</i> , 2006, 91, 3390-3396.	0.2	15
22	The Dewetting Transition and The Hydrophobic Effect. <i>Journal of the American Chemical Society</i> , 2007, 129, 4847-4852.	6.6	139
23	Role of Flexibility and Polarity as Determinants of the Hydration of Internal Cavities and Pockets in Proteins. <i>Biophysical Journal</i> , 2007, 93, 2791-2804.	0.2	38
24	Heat capacity changes upon burial of polar and nonpolar groups in proteins. <i>Protein Science</i> , 2008, 10, 1343-1352.	3.1	120
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26	Crystallographic Study of Hydration of an Internal Cavity in Engineered Proteins with Buried Polar or Ionizable Groups. <i>Biophysical Journal</i> , 2008, 94, 3208-3216.	0.2	28
27	Dynamics at the Protein-Water Interface from 17O Spin Relaxation in Deeply Supercooled Solutions. <i>Biophysical Journal</i> , 2008, 95, 2951-2963.	0.2	132
28	Minimizing frustration by folding in an aqueous environment. <i>Archives of Biochemistry and Biophysics</i> , 2008, 469, 118-131.	1.4	18
29	Glutamic acid 242 is a valve in the proton pump of cytochrome <i>c</i> oxidase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 6255-6259.	3.3	125
30	Structural coupling between FKBP12 and buried water. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 74, 603-611.	1.5	63
31	Computations of Standard Binding Free Energies with Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2009, 113, 2234-2246.	1.2	481
32	Hydrated and Dehydrated Tertiary Interactionsâ€œOpening and Closingâ€œ of a Four-Helix Bundle Peptide. <i>Biophysical Journal</i> , 2009, 97, 572-580.	0.2	2
33	Structural and dynamic properties of water around acetylcholinesterase. <i>Protein Science</i> , 2009, 11, 2080-2090.	3.1	95
34	Water in the Polar and Nonpolar Cavities of the Protein Interleukin-1Î². <i>Journal of Physical Chemistry B</i> , 2010, 114, 16290-16297.	1.2	39
35	Molecular Dynamics Free Energy Calculations to Assess the Possibility of Water Existence in Protein Nonpolar Cavities. <i>Biophysical Journal</i> , 2010, 98, 2974-2983.	0.2	10
36	Simulations of the confinement of ubiquitin in self-assembled reverse micelles. <i>Journal of Chemical Physics</i> , 2011, 134, 225101.	1.2	54

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37	Water in the Active Site of Ketosteroid Isomerase. <i>Biochemistry</i> , 2011, 50, 6689-6700.	1.2	7
38	Comparative void-volume analysis of psychrophilic and mesophilic enzymes: Structural bioinformatics of psychrophilic enzymes reveals sources of core flexibility. <i>BMC Structural Biology</i> , 2011, 11, 42.	2.3	67
39	The Role of Conserved Waters in Conformational Transitions of Q61H K-ras. <i>PLoS Computational Biology</i> , 2012, 8, e1002394.	1.5	48
40	Early Turn Formation and Chain Collapse Drive Fast Folding of the Major Cold Shock Protein CspA of <i>Escherichia coli</i> . <i>Biochemistry</i> , 2012, 51, 9104-9111.	1.2	20
41	The effect of protein composition on hydration dynamics. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3570.	1.3	25
42	Thermodynamic framework for identifying free energy inventories of enzyme catalytic cycles. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 12271-12276.	3.3	13
43	Interaction of Amyloid Inhibitor Proteins with Amyloid Beta Peptides: Insight from Molecular Dynamics Simulations. <i>PLoS ONE</i> , 2014, 9, e113041.	1.1	40
44	Water Dynamics in Protein Hydration Shells: The Molecular Origins of the Dynamical Perturbation. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7715-7729.	1.2	207
45	Stay Wet, Stay Stable? How Internal Water Helps the Stability of Thermophilic Proteins. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12760-12770.	1.2	21
46	Role of Internal Water on Protein Thermal Stability: The Case of Homologous G Domains. <i>Journal of Physical Chemistry B</i> , 2015, 119, 8939-8949.	1.2	21
47	Effect of Glycosylation on an Immunodominant Region in the V1V2 Variable Domain of the HIV-1 Envelope gp120 Protein. <i>PLoS Computational Biology</i> , 2016, 12, e1005094.	1.5	17
48	Water Determines the Structure and Dynamics of Proteins. <i>Chemical Reviews</i> , 2016, 116, 7673-7697.	23.0	645
49	Water Dynamics in the Hydration Shells of Biomolecules. <i>Chemical Reviews</i> , 2017, 117, 10694-10725.	23.0	574
50	In Silico Studies of Small Molecule Interactions with Enzymes Reveal Aspects of Catalytic Function. <i>Catalysts</i> , 2017, 7, 212.	1.6	21