

Volkhard Helms

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89
papers

2,971
citations

29
h-index

52
g-index

100
ext. papers

3,430
ext. citations

5.3
avg, IF

5.24
L-index

#	Paper	IF	Citations
89	The mechanism of proton exclusion in the aquaporin-1 water channel. <i>Journal of Molecular Biology</i> , 2003 , 333, 279-93	6.5	233
88	Transient pockets on protein surfaces involved in protein-protein interaction. <i>Journal of Medicinal Chemistry</i> , 2007 , 50, 3457-64	8.3	189
87	NWChem: Past, present, and future. <i>Journal of Chemical Physics</i> , 2020 , 152, 184102	3.9	187
86	Proton shuttle in green fluorescent protein studied by dynamic simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 2778-81	11.5	131
85	Diffusional encounter of barnase and barstar. <i>Biophysical Journal</i> , 2006 , 90, 1913-24	2.9	112
84	BiP-mediated closing of the Sec61 channel limits Ca ²⁺ leakage from the ER. <i>EMBO Journal</i> , 2012 , 31, 3282-96	13	111
83	Atomistic simulation of water percolation and proton hopping in Nafion fuel cell membrane. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 13681-90	3.4	108
82	Protein dynamics tightly connected to the dynamics of surrounding and internal water molecules. <i>ChemPhysChem</i> , 2007 , 8, 23-33	3.2	85
81	Computational Alchemy To Calculate Absolute Protein-Ligand Binding Free Energy. <i>Journal of the American Chemical Society</i> , 1998 , 120, 2710-2713	16.4	84
80	Molecular dynamics simulation of proton transport with quantum mechanically derived proton hopping rates (Q-HOP MD). <i>Journal of Chemical Physics</i> , 2001 , 115, 7993-8005	3.9	80
79	Statistical analysis of predominantly transient protein-protein interfaces. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005 , 61, 344-55	4.2	71
78	Low-lying electronic excitations of the green fluorescent protein chromophore. <i>Computational and Theoretical Chemistry</i> , 2000 , 506, 179-189		71
77	Interaction of calmodulin with Sec61-limits Ca ²⁺ leakage from the endoplasmic reticulum. <i>EMBO Journal</i> , 2011 , 30, 17-31	13	70
76	Mechanism of fast peptide recognition by SH3 domains. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 7626-30	16.4	66
75	Protein transport into the human endoplasmic reticulum. <i>Journal of Molecular Biology</i> , 2015 , 427, 1159-75		55
74	Cyclophilin A binds to linear peptide motifs containing a consensus that is present in many human proteins. <i>Journal of Biological Chemistry</i> , 2005 , 280, 23668-74	5.4	55
73	Tandem repeats in the CpG islands of imprinted genes. <i>Genomics</i> , 2006 , 88, 323-32	4.3	52

72	What induces pocket openings on protein surface patches involved in protein-protein interactions?. <i>Journal of Computer-Aided Molecular Design</i> , 2009 , 23, 73-86	4.2	49
71	TFmiR: a web server for constructing and analyzing disease-specific transcription factor and miRNA co-regulatory networks. <i>Nucleic Acids Research</i> , 2015 , 43, W283-8	20.1	43
70	Attraction within the membrane. Forces behind transmembrane protein folding and supramolecular complex assembly. <i>EMBO Reports</i> , 2002 , 3, 1133-8	6.5	43
69	AXER is an ATP/ADP exchanger in the membrane of the endoplasmic reticulum. <i>Nature Communications</i> , 2018 , 9, 3489	17.4	42
68	Conserved gating elements in TRPC4 and TRPC5 channels. <i>Journal of Biological Chemistry</i> , 2013 , 288, 19471-83	5.4	40
67	A spatial model of the chromatophore vesicles of <i>Rhodobacter sphaeroides</i> and the position of the Cytochrome bc1 complex. <i>Biophysical Journal</i> , 2006 , 91, 921-6	2.9	40
66	Proteomics reveals signal peptide features determining the client specificity in human TRAP-dependent ER protein import. <i>Nature Communications</i> , 2018 , 9, 3765	17.4	37
65	Reconstruction of a kinetic model of the chromatophore vesicles from <i>Rhodobacter sphaeroides</i> . <i>Biophysical Journal</i> , 2006 , 91, 927-37	2.9	36
64	Fatty acid elongation in non-alcoholic steatohepatitis and hepatocellular carcinoma. <i>International Journal of Molecular Sciences</i> , 2014 , 15, 5762-73	6.3	35
63	Free Energy Landscape of Protein-Protein Encounter Resulting from Brownian Dynamics Simulations of Barnase:Barstar. <i>Journal of Chemical Theory and Computation</i> , 2005 , 1, 723-36	6.4	35
62	Compact parameter set for fast estimation of proton transfer rates. <i>Journal of Chemical Physics</i> , 2001 , 114, 1125-1132	3.9	33
61	A structural model of the complex formed by phospholamban and the calcium pump of sarcoplasmic reticulum obtained by molecular mechanics. <i>ChemBioChem</i> , 2002 , 3, 1200-8	3.8	31
60	Titration behavior of residues at the entrance of the D-pathway of cytochrome c oxidase from <i>paracoccus denitrificans</i> investigated by continuum electrostatic calculations. <i>Biophysical Journal</i> , 2005 , 89, 2324-31	2.9	29
59	Brownian dynamics simulations of simplified cytochrome c molecules in the presence of a charged surface. <i>Journal of Chemical Physics</i> , 2004 , 121, 457-64	3.9	27
58	Reaction rates for proton transfer over small barriers and connection to transition state theory. <i>Journal of Chemical Physics</i> , 2001 , 115, 7985-7992	3.9	27
57	PreTIS: A Tool to Predict Non-canonical 5TUTR Translational Initiation Sites in Human and Mouse. <i>PLoS Computational Biology</i> , 2016 , 12, e1005170	5	27
56	Matched-cohort DNA microarray diversity analysis of methicillin sensitive and methicillin resistant <i>Staphylococcus aureus</i> isolates from hospital admission patients. <i>PLoS ONE</i> , 2012 , 7, e52487	3.7	26
55	Druggability of dynamic protein-protein interfaces. <i>Current Pharmaceutical Design</i> , 2012 , 18, 4599-606	3.3	26

54	DNA co-methylation analysis suggests novel functional associations between gene pairs in breast cancer samples. <i>Human Molecular Genetics</i> , 2013 , 22, 3016-22	5.6	24
53	Identification of key player genes in gene regulatory networks. <i>BMC Systems Biology</i> , 2016 , 10, 88	3.5	23
52	TMBHMM: a frequency profile based HMM for predicting the topology of transmembrane beta barrel proteins and the exposure status of transmembrane residues. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011 , 1814, 664-70	4	23
51	Novel scoring function for modeling structures of oligomers of transmembrane alpha-helices. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004 , 57, 577-85	4.2	22
50	Energetics of Hydrophilic Protein-Protein Association and the Role of Water. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3512-24	6.4	21
49	Community-Associated Staphylococcus aureus from Sub-Saharan Africa and Germany: A Cross-Sectional Geographic Correlation Study. <i>Scientific Reports</i> , 2017 , 7, 154	4.9	20
48	Are solvation free energies of homogeneous helical peptides additive?. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 19000-7	3.4	20
47	Multicopy molecular dynamics simulations suggest how to reconcile crystallographic and product formation data for camphor enantiomers bound to cytochrome P-450cam. <i>Journal of Inorganic Biochemistry</i> , 2000 , 81, 121-31	4.2	20
46	Energetics of liposomes encapsulating silica nanoparticles. <i>Journal of Molecular Modeling</i> , 2013 , 19, 2459-72	19	
45	Downhill binding energy surface of the barnase-barstar complex. <i>Biopolymers</i> , 2010 , 93, 977-85	2.2	19
44	Interfacing Brownian dynamics simulations. <i>Journal of Chemical Physics</i> , 2004 , 120, 4573-80	3.9	19
43	Putative cholesterol-binding sites in human immunodeficiency virus (HIV) coreceptors CXCR4 and CCR5. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013 , 81, 555-67	4.2	18
42	Polyamines: naturally occurring small molecule modulators of electrostatic protein-protein interactions. <i>Journal of Inorganic Biochemistry</i> , 2010 , 104, 118-25	4.2	18
41	Tightly connected water wires facilitate fast proton uptake at the proton entrance of proton pumping proteins. <i>Journal of the American Chemical Society</i> , 2009 , 131, 2080-1	16.4	17
40	Lanthanum ions inhibit the mammalian Sec61 complex in its channel dynamics and protein transport activity. <i>FEBS Letters</i> , 2009 , 583, 2359-64	3.8	17
39	The mRNA-binding Protein TTP/ZFP36 in Hepatocarcinogenesis and Hepatocellular Carcinoma. <i>Cancers</i> , 2019 , 11,	6.6	16
38	Dynamic protonation equilibrium of solvated acetic acid. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 2939-43	16.4	16
37	BEclear: Batch Effect Detection and Adjustment in DNA Methylation Data. <i>PLoS ONE</i> , 2016 , 11, e0159923	17	16

36	Classifying substrate specificities of membrane transporters from <i>Arabidopsis thaliana</i> . <i>Journal of Chemical Information and Modeling</i> , 2010 , 50, 1899-905	6.1	14
35	How strongly do sequence conservation patterns and empirical scales correlate with exposure patterns of transmembrane helices of membrane proteins?. <i>Biopolymers</i> , 2006 , 83, 389-99	2.2	14
34	Dynamical binding of proline-rich peptides to their recognition domains. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2005 , 1754, 232-8	4	14
33	ALLO: A tool to discriminate and prioritize allosteric pockets. <i>Chemical Biology and Drug Design</i> , 2018 , 91, 845-853	2.9	13
32	Rule-based regulatory and metabolic model for Quorum sensing in <i>P. aeruginosa</i> . <i>BMC Systems Biology</i> , 2013 , 7, 81	3.5	13
31	Assembly of transmembrane helices of simple polytopic membrane proteins from sequence conservation patterns. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006 , 64, 895-905	4.2	13
30	Transferring functional annotations of membrane transporters on the basis of sequence similarity and sequence motifs. <i>BMC Bioinformatics</i> , 2013 , 14, 343	3.6	12
29	Functional classification of membrane transporters and channels based on filtered TM/non-TM amino acid composition. <i>Biopolymers</i> , 2012 , 97, 558-67	2.2	12
28	SNP and indel frequencies at transcription start sites and at canonical and alternative translation initiation sites in the human genome. <i>PLoS ONE</i> , 2019 , 14, e0214816	3.7	11
27	Design of a gated molecular proton channel. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 768-716.4	6.4	11
26	Transient pockets on XIAP-BIR2: toward the characterization of putative binding sites of small-molecule XIAP inhibitors. <i>Journal of Molecular Modeling</i> , 2012 , 18, 2031-42	2	10
25	Identifying continuous pores in protein structures with PROPORES by computational repositioning of gating residues. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012 , 80, 421-32	4.2	9
24	Contribution of charged and polar residues for the formation of the E1-E2 heterodimer from Hepatitis C Virus. <i>Journal of Molecular Modeling</i> , 2010 , 16, 1625-37	2	9
23	Mechanism of phosphoryl transfer in kinases investigated by semiempirical calculations. <i>International Journal of Quantum Chemistry</i> , 2003 , 95, 479-486	2.1	9
22	Cellular functions of genetically imprinted genes in human and mouse as annotated in the gene ontology. <i>PLoS ONE</i> , 2012 , 7, e50285	3.7	8
21	TRAM1 protein may support ER protein import by modulating the phospholipid bilayer near the lateral gate of the Sec61-channel. <i>Channels</i> , 2020 , 14, 28-44	3	6
20	Linking Hematopoietic Differentiation to Co-Expressed Sets of Pluripotency-Associated and Imprinted Genes and to Regulatory microRNA-Transcription Factor Motifs. <i>PLoS ONE</i> , 2017 , 12, e0166852	3.7	6
19	Relative Principal Components Analysis: Application to Analyzing Biomolecular Conformational Changes. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 2166-2178	6.4	5

18	Batch tautomer generation with MolTPC. <i>Journal of Computational Chemistry</i> , 2013 , 34, 2485-92	3.5	5
17	Statistical analysis and exposure status classification of transmembrane beta barrel residues. <i>Computational Biology and Chemistry</i> , 2011 , 35, 96-107	3.6	5
16	Different protonation equilibria of 4-methylimidazole and acetic acid. <i>ChemPhysChem</i> , 2007 , 8, 2445-51	3.2	5
15	Molecular dynamics simulation of truncated bovine adrenodoxin. <i>Biopolymers</i> , 2005 , 78, 9-20	2.2	5
14	Helical integrity and microsolvation of transmembrane domains from Flaviviridae envelope glycoproteins. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2011 , 1808, 1040-9	3.8	4
13	Detection of Acidic Pharmaceutical Compounds Using Virus-Based Molecularly Imprinted Polymers. <i>Polymers</i> , 2018 , 10,	4.5	4
12	Prediction of Synergistic Toxicity of Binary Mixtures to <i>Vibrio fischeri</i> Based on Biomolecular Interaction Networks. <i>Chemical Research in Toxicology</i> , 2018 , 31, 1138-1150	4	3
11	Methylation-targeted specificity of the DNA binding proteins R.DpnI and MeCP2 studied by molecular dynamics simulations. <i>Journal of Molecular Modeling</i> , 2017 , 23, 152	2	2
10	Topology Consistency of Disease-specific Differential Co-regulatory Networks. <i>BMC Bioinformatics</i> , 2019 , 20, 550	3.6	2
9	Elucidating the energetic contributions to the binding free energy. <i>Journal of Chemical Physics</i> , 2017 , 146, 014105	3.9	2
8	How does Sec63 affect the conformation of Sec61 in yeast?. <i>PLoS Computational Biology</i> , 2021 , 17, e1008855	3.8	2
7	Graph-theoretical identification of dissociation pathways on free energy landscapes of biomolecular interaction. <i>Journal of Computational Chemistry</i> , 2010 , 31, 847-54	3.5	1
6	Interorganelle Tethering to Endocytic Organelles Determines Directional Cytokine Transport in CD4 T Cells. <i>Journal of Immunology</i> , 2020 , 205, 2988-3000	5.3	1
5	ProPores2: Web Service and Stand-Alone Tool for Identifying, Manipulating, and Visualizing Pores in Protein Structures. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 1555-1559	6.1	1
4	Quantitative Proteomics and Differential Protein Abundance Analysis after Depletion of Putative mRNA Receptors in the ER Membrane of Human Cells Identifies Novel Aspects of mRNA Targeting to the ER. <i>Molecules</i> , 2021 , 26,	4.8	1
3	TopControl: A Tool to Prioritize Candidate Disease-associated Genes based on Topological Network Features. <i>Scientific Reports</i> , 2019 , 9, 19472	4.9	1
2	A longer isoform of Stim1 is a negative SOCE regulator but increases cAMP-modulated NFAT signaling.. <i>EMBO Reports</i> , 2021 , e53135	6.5	1
1	A Methylation-Directed, Synthetic Pap Switch Based on Self-Complementary Regulatory DNA Reconstituted in an All Cell-Free Expression System. <i>ACS Synthetic Biology</i> , 2021 , 10, 2725-2739	5.7	

