Volkhard Helms

List of Publications by Year in Descending Order

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	How does Sec63 affect the conformation of Sec61 in yeast?. *PLoS Computational Biology*, **2021**, 17, e1008855	3	2
88	ProPores2: Web Service and Stand-Alone Tool for Identifying, Manipulating, and Visualizing Pores in Protein Structures. *Journal of Chemical Information and Modeling*, **2021**, 61, 1555-1559	6.1	1
87	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. *Molecules*, **2021**, 26,	4.8	1
86	A Methylation-Directed, Synthetic Pap Switch Based on Self-Complementary Regulatory DNA Reconstituted in an All Cell-Free Expression System. *ACS Synthetic Biology*, **2021**, 10, 2725-2739	5.7	
85	A longer isoform of Stim1 is a negative SOCE regulator but increases cAMP-modulated NFAT signaling.. *EMBO Reports*, **2021**, e53135	6.5	1
84	NWChem: Past, present, and future. *Journal of Chemical Physics*, **2020**, 152, 184102	3.9	187
83	TRAM1 protein may support ER protein import by modulating the phospholipid bilayer near the lateral gate of the Sec61-channel. *Channels*, **2020**, 14, 28-44	3	6
82	Interorganelle Tethering to Endocytic Organelles Determines Directional Cytokine Transport in CD4 T Cells. *Journal of Immunology*, **2020**, 205, 2988-3000	5.3	1
81	SNP and indel frequencies at transcription start sites and at canonical and alternative translation initiation sites in the human genome. *PLoS ONE*, **2019**, 14, e0214816	3.7	11
80	Relative Principal Components Analysis: Application to Analyzing Biomolecular Conformational Changes. *Journal of Chemical Theory and Computation*, **2019**, 15, 2166-2178	6.4	5
79	Topology Consistency of Disease-specific Differential Co-regulatory Networks. *BMC Bioinformatics*, **2019**, 20, 550	3.6	2
78	The mRNA-binding Protein TTP/ZFP36 in Hepatocarcinogenesis and Hepatocellular Carcinoma. *Cancers*, **2019**, 11,	6.6	16
77	TopControl: A Tool to Prioritize Candidate Disease-associated Genes based on Topological Network Features. *Scientific Reports*, **2019**, 9, 19472	4.9	1
76	ALLO: A tool to discriminate and prioritize allosteric pockets. *Chemical Biology and Drug Design*, **2018**, 91, 845-853	2.9	13
75	Prediction of Synergistic Toxicity of Binary Mixtures to Vibrio fischeri Based on Biomolecular Interaction Networks. *Chemical Research in Toxicology*, **2018**, 31, 1138-1150	4	3
74	Proteomics reveals signal peptide features determining the client specificity in human TRAP-dependent ER protein import. *Nature Communications*, **2018**, 9, 3765	17.4	37
73	Detection of Acidic Pharmaceutical Compounds Using Virus-Based Molecularly Imprinted Polymers. *Polymers*, **2018**, 10,	4.5	4

72	AXER is an ATP/ADP exchanger in the membrane of the endoplasmic reticulum. *Nature Communications*, **2018**, 9, 3489	17.4	42
71	Community-Associated Staphylococcus aureus from Sub-Saharan Africa and Germany: A Cross-Sectional Geographic Correlation Study. *Scientific Reports*, **2017**, 7, 154	4.9	20
70	Methylation-targeted specificity of the DNA binding proteins R.DpnI and MeCP2 studied by molecular dynamics simulations. *Journal of Molecular Modeling*, **2017**, 23, 152	2	2
69	Linking Hematopoietic Differentiation to Co-Expressed Sets of Pluripotency-Associated and Imprinted Genes and to Regulatory microRNA-Transcription Factor Motifs. *PLoS ONE*, **2017**, 12, e0166852	3.7	6
68	Elucidating the energetic contributions to the binding free energy. *Journal of Chemical Physics*, **2017**, 146, 014105	3.9	2
67	Identification of key player genes in gene regulatory networks. *BMC Systems Biology*, **2016**, 10, 88	3.5	23
66	BEclear: Batch Effect Detection and Adjustment in DNA Methylation Data. *PLoS ONE*, **2016**, 11, e0159921	3.7	16
65	PreTIS: A Tool to Predict Non-canonical 5TUTR Translational Initiation Sites in Human and Mouse. *PLoS Computational Biology*, **2016**, 12, e1005170	5	27
64	Protein transport into the human endoplasmic reticulum. *Journal of Molecular Biology*, **2015**, 427, 1159-75	6.5	55
63	TFmiR: a web server for constructing and analyzing disease-specific transcription factor and miRNA co-regulatory networks. *Nucleic Acids Research*, **2015**, 43, W283-8	20.1	43
62	Energetics of Hydrophilic Protein-Protein Association and the Role of Water. *Journal of Chemical Theory and Computation*, **2014**, 10, 3512-24	6.4	21
61	Fatty acid elongation in non-alcoholic steatohepatitis and hepatocellular carcinoma. *International Journal of Molecular Sciences*, **2014**, 15, 5762-73	6.3	35
60	Energetics of liposomes encapsulating silica nanoparticles. *Journal of Molecular Modeling*, **2013**, 19, 2459-72	2	19
59	Rule-based regulatory and metabolic model for Quorum sensing in P. aeruginosa. *BMC Systems Biology*, **2013**, 7, 81	3.5	13
58	Transferring functional annotations of membrane transporters on the basis of sequence similarity and sequence motifs. *BMC Bioinformatics*, **2013**, 14, 343	3.6	12
57	Batch tautomer generation with MolTPC. *Journal of Computational Chemistry*, **2013**, 34, 2485-92	3.5	5
56	DNA co-methylation analysis suggests novel functional associations between gene pairs in breast cancer samples. *Human Molecular Genetics*, **2013**, 22, 3016-22	5.6	24
55	Putative cholesterol-binding sites in human immunodeficiency virus (HIV) coreceptors CXCR4 and CCR5. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 555-67	4.2	18

54	Conserved gating elements in TRPC4 and TRPC5 channels. *Journal of Biological Chemistry*, **2013**, 288, 19471-83	5.4	40
53	Matched-cohort DNA microarray diversity analysis of methicillin sensitive and methicillin resistant Staphylococcus aureus isolates from hospital admission patients. *PLoS ONE*, **2012**, 7, e52487	3.7	26
52	Identifying continuous pores in protein structures with PROPORES by computational repositioning of gating residues. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 421-32	4.2	9
51	Functional classification of membrane transporters and channels based on filtered TM/non-TM amino acid composition. *Biopolymers*, **2012**, 97, 558-67	2.2	12
50	Transient pockets on XIAP-BIR2: toward the characterization of putative binding sites of small-molecule XIAP inhibitors. *Journal of Molecular Modeling*, **2012**, 18, 2031-42	2	10
49	BiP-mediated closing of the Sec61 channel limits Ca2+ leakage from the ER. *EMBO Journal*, **2012**, 31, 3282-96	13	111
48	Druggability of dynamic protein-protein interfaces. *Current Pharmaceutical Design*, **2012**, 18, 4599-606	3.3	26
47	Cellular functions of genetically imprinted genes in human and mouse as annotated in the gene ontology. *PLoS ONE*, **2012**, 7, e50285	3.7	8
46	Helical integrity and microsolvation of transmembrane domains from Flaviviridae envelope glycoproteins. *Biochimica Et Biophysica Acta - Biomembranes*, **2011**, 1808, 1040-9	3.8	4
45	Interaction of calmodulin with Sec61 limits Ca2+ leakage from the endoplasmic reticulum. *EMBO Journal*, **2011**, 30, 17-31	13	70
44	Design of a gated molecular proton channel. *Angewandte Chemie - International Edition*, **2011**, 50, 768-71	16.4	11
43	Statistical analysis and exposure status classification of transmembrane beta barrel residues. *Computational Biology and Chemistry*, **2011**, 35, 96-107	3.6	5
42	TMBHMM: a frequency profile based HMM for predicting the topology of transmembrane beta barrel proteins and the exposure status of transmembrane residues. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2011**, 1814, 664-70	4	23
41	Atomistic simulation of water percolation and proton hopping in Nafion fuel cell membrane. *Journal of Physical Chemistry B*, **2010**, 114, 13681-90	3.4	108
40	Classifying substrate specificities of membrane transporters from Arabidopsis thaliana. *Journal of Chemical Information and Modeling*, **2010**, 50, 1899-905	6.1	14
39	Graph-theoretical identification of dissociation pathways on free energy landscapes of biomolecular interaction. *Journal of Computational Chemistry*, **2010**, 31, 847-54	3.5	1
38	Contribution of charged and polar residues for the formation of the E1-E2 heterodimer from Hepatitis C Virus. *Journal of Molecular Modeling*, **2010**, 16, 1625-37	2	9
37	Downhill binding energy surface of the barnase-barstar complex. *Biopolymers*, **2010**, 93, 977-85	2.2	19

36	Polyamines: naturally occurring small molecule modulators of electrostatic protein-protein interactions. *Journal of Inorganic Biochemistry*, **2010**, 104, 118-25	4.2	18
35	Tightly connected water wires facilitate fast proton uptake at the proton entrance of proton pumping proteins. *Journal of the American Chemical Society*, **2009**, 131, 2080-1	16.4	17
34	Lanthanum ions inhibit the mammalian Sec61 complex in its channel dynamics and protein transport activity. *FEBS Letters*, **2009**, 583, 2359-64	3.8	17
33	What induces pocket openings on protein surface patches involved in protein-protein interactions?. *Journal of Computer-Aided Molecular Design*, **2009**, 23, 73-86	4.2	49
32	Mechanism of fast peptide recognition by SH3 domains. *Angewandte Chemie - International Edition*, **2008**, 47, 7626-30	16.4	66
31	Transient pockets on protein surfaces involved in protein-protein interaction. *Journal of Medicinal Chemistry*, **2007**, 50, 3457-64	8.3	189
30	Dynamic protonation equilibrium of solvated acetic acid. *Angewandte Chemie - International Edition*, **2007**, 46, 2939-43	16.4	16
29	Protein dynamics tightly connected to the dynamics of surrounding and internal water molecules. *ChemPhysChem*, **2007**, 8, 23-33	3.2	85
28	Different protonation equilibria of 4-methylimidazole and acetic acid. *ChemPhysChem*, **2007**, 8, 2445-51	3.2	5
27	How strongly do sequence conservation patterns and empirical scales correlate with exposure patterns of transmembrane helices of membrane proteins?. *Biopolymers*, **2006**, 83, 389-99	2.2	14
26	Reconstruction of a kinetic model of the chromatophore vesicles from Rhodobacter sphaeroides. *Biophysical Journal*, **2006**, 91, 927-37	2.9	36
25	Diffusional encounter of barnase and barstar. *Biophysical Journal*, **2006**, 90, 1913-24	2.9	112
24	A spatial model of the chromatophore vesicles of Rhodobacter sphaeroides and the position of the Cytochrome bc1 complex. *Biophysical Journal*, **2006**, 91, 921-6	2.9	40
23	Tandem repeats in the CpG islands of imprinted genes. *Genomics*, **2006**, 88, 323-32	4.3	52
22	Assembly of transmembrane helices of simple polytopic membrane proteins from sequence conservation patterns. *Proteins: Structure, Function and Bioinformatics*, **2006**, 64, 895-905	4.2	13
21	Are solvation free energies of homogeneous helical peptides additive?. *Journal of Physical Chemistry B*, **2005**, 109, 19000-7	3.4	20
20	Free Energy Landscape of Protein-Protein Encounter Resulting from Brownian Dynamics Simulations of Barnase:Barstar. *Journal of Chemical Theory and Computation*, **2005**, 1, 723-36	6.4	35
19	Titration behavior of residues at the entrance of the D-pathway of cytochrome c oxidase from paracoccus denitrificans investigated by continuum electrostatic calculations. *Biophysical Journal*, **2005**, 89, 2324-31	2.9	29

18	Dynamical binding of proline-rich peptides to their recognition domains. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2005**, 1754, 232-8	4	14
17	Molecular dynamics simulation of truncated bovine adrenodoxin. *Biopolymers*, **2005**, 78, 9-20	2.2	5
16	Statistical analysis of predominantly transient protein-protein interfaces. *Proteins: Structure, Function and Bioinformatics*, **2005**, 61, 344-55	4.2	71
15	Cyclophilin A binds to linear peptide motifs containing a consensus that is present in many human proteins. *Journal of Biological Chemistry*, **2005**, 280, 23668-74	5.4	55
14	Interfacing Brownian dynamics simulations. *Journal of Chemical Physics*, **2004**, 120, 4573-80	3.9	19
13	Brownian dynamics simulations of simplified cytochrome c molecules in the presence of a charged surface. *Journal of Chemical Physics*, **2004**, 121, 457-64	3.9	27
12	Novel scoring function for modeling structures of oligomers of transmembrane alpha-helices. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 577-85	4.2	22
11	Mechanism of phosphoryl transfer in kinases investigated by semiempirical calculations. *International Journal of Quantum Chemistry*, **2003**, 95, 479-486	2.1	9
10	The mechanism of proton exclusion in the aquaporin-1 water channel. *Journal of Molecular Biology*, **2003**, 333, 279-93	6.5	233
9	A structural model of the complex formed by phospholamban and the calcium pump of sarcoplasmic reticulum obtained by molecular mechanics. *ChemBioChem*, **2002**, 3, 1200-8	3.8	31
8	Attraction within the membrane. Forces behind transmembrane protein folding and supramolecular complex assembly. *EMBO Reports*, **2002**, 3, 1133-8	6.5	43
7	Proton shuttle in green fluorescent protein studied by dynamic simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 2778-81	11.5	131
6	Reaction rates for proton transfer over small barriers and connection to transition state theory. *Journal of Chemical Physics*, **2001**, 115, 7985-7992	3.9	27
5	Compact parameter set for fast estimation of proton transfer rates. *Journal of Chemical Physics*, **2001**, 114, 1125-1132	3.9	33
4	Molecular dynamics simulation of proton transport with quantum mechanically derived proton hopping rates (Q-HOP MD). *Journal of Chemical Physics*, **2001**, 115, 7993-8005	3.9	80
3	Multicopy molecular dynamics simulations suggest how to reconcile crystallographic and product formation data for camphor enantiomers bound to cytochrome P-450cam. *Journal of Inorganic Biochemistry*, **2000**, 81, 121-31	4.2	20
2	Low-lying electronic excitations of the green fluorescent protein chromophore. *Computational and Theoretical Chemistry*, **2000**, 506, 179-189		71
1	Computational Alchemy To Calculate Absolute Protein□ligand Binding Free Energy. *Journal of the American Chemical Society*, **1998**, 120, 2710-2713	16.4	84