Marc W Van Der Kamp

List of Publications by Year
in descending order

79 papers	3,191 citations	159358 30 h-index	174990 52 g-index
94 all docs	94 docs citations	94 times ranked	4443 citing authors

#	Article	IF	Citations
1	Combined Quantum Mechanics/Molecular Mechanics (QM/MM) Methods in Computational Enzymology. Biochemistry, 2013, 52, 2708-2728.	1.2	471
2	On the Temperature Dependence of Enzyme-Catalyzed Rates. Biochemistry, 2016, 55, 1681-1688.	1.2	233
3	The Catalytic Mechanism of a Natural Dielsâ€“Alderase Revealed in Molecular Detail. Journal of the American Chemical Society, 2016, 138, 6095-6098.	6.6	146
4	Dynameomics: A Comprehensive Database of Protein Dynamics. Structure, 2010, 18, 423-435.	1.6	131
5	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1393.	6.2	110
6	Pathogenic Mutations in the Hydrophobic Core of the Human Prion Protein Can Promote Structural Instability and Misfolding. Journal of Molecular Biology, 2010, 404, 732-748.	2.0	99
7	Biomolecular simulation and modelling: status, progress and prospects. Journal of the Royal Society Interface, 2008, 5, 173-190.	1.5	77
8	The Basis for Carbapenem Hydrolysis by Class A Î²-Lactamases: A Combined Investigation using Crystallography and Simulations. Journal of the American Chemical Society, 2012, 134, 18275-18285.	6.6	76
9	Influence of pH on the Human Prion Protein: Insights into the Early Steps ofÂMisfolding. Biophysical Journal, 2010, 99, 2289-2298.	0.2	75
10	The consequences of pathogenic mutations to the human prion protein. Protein Engineering, Design and Selection, 2009, 22, 461-468.	1.0	73
11	Atomistic non-adiabatic dynamics of the LH2 complex with a GPU-accelerated ab initio exciton model. Physical Chemistry Chemical Physics, 2017, 19, 14924-14936.	1.3	64
12	Dynamical origins of heat capacity changes in enzyme-catalysed reactions. Nature Communications, 2018, 9, 1177.	5.8	64
13	Loop Motion in Triosephosphate Isomerase Is Not a Simple Open and Shut Case. Journal of the American Chemical Society, 2018, 140, 15889-15903.	6.6	63
14	Testing High-Level QM/MM Methods for Modeling Enzyme Reactions: Acetyl-CoA Deprotonation in Citrate Synthase. Journal of Physical Chemistry B, 2010, 114, 11303-11314.	1.2	61
15	Evolution of dynamical networks enhances catalysis in a designer enzyme. Nature Chemistry, 2021, 13, 1017-1022.	6.6	60
16	A Projector-Embedding Approach for Multiscale Coupled-Cluster Calculations Applied to Citrate Synthase. Journal of Chemical Theory and Computation, 2016, 12, 2689-2697.	2.3	58
17	Comparison of ab Initio, DFT, and Semiempirical QM/MM Approaches for Description of Catalytic Mechanism of Hairpin Ribozyme. Journal of Chemical Theory and Computation, 2014, 10, 1608-1622.	2.3	56
18	Enzyme evolution and the temperature dependence of enzyme catalysis. Current Opinion in Structural Biology, 2020, 65, 96-101.	2.6	54

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19	Computational enzymology: insight into biological catalysts from modelling. Natural Product Reports, 2008, 25, 1001.	5.2	51
20	Specificity of bispecific T cell receptors and antibodies targeting peptide-HLA. Journal of Clinical Investigation, 2020, 130, 2673-2688.	3.9	50
21	Structural Basis of Catalysis in the Bacterial Monoterpene Synthases Linalool Synthase and 1,8-Cineole Synthase. ACS Catalysis, 2017, 7, 6268-6282.	5.5	47
22	QM/MM simulations as an assay for carbapenemase activity in class A Î²-lactamases. Chemical Communications, 2014, 50, 14736-14739.	2.2	43
23	Loop Dynamics and Enzyme Catalysis in Protein Tyrosine Phosphatases. Journal of the American Chemical Society, 2021, 143, 3830-3845.	6.6	42
24	Reaction Mechanism of N-Acetylneuraminic Acid Lyase Revealed by a Combination of Crystallography, QM/MM Simulation, and Mutagenesis. ACS Chemical Biology, 2014, 9, 1025-1032.	1.6	41
25	High-level QM/MM modelling predicts an arginine as the acid in the condensation reaction catalysed by citrate synthase. Chemical Communications, 2008, , 1874.	2.2	39
26	Diverse Effects on the Native Î²-Sheet of the Human Prion Protein Due to Disease-Associated Mutations. Biochemistry, 2010, 49, 9874-9881.	1.2	38
27	QM/<scp>MM</scp> modelling of ketosteroid isomerase reactivity indicates that active site closure is integral to catalysis. FEBS Journal, 2013, 280, 3120-3131.	2.2	34
28	Comparison of Different Quantum Mechanical/Molecular Mechanics Boundary Treatments in the Reaction of the Hepatitis C Virus NS3 Protease with the NS5A/5B Substrate. Journal of Physical Chemistry B, 2007, 111, 12909-12915.	1.2	32
29	Experiment and Simulation Reveal How Mutations in Functional Plasticity Regions Guide Plant Monoterpene Synthase Product Outcome. ACS Catalysis, 2018, 8, 3780-3791.	5.5	32
30	Structural and Dynamic Properties of the Human Prion Protein. Biophysical Journal, 2014, 106, 1152-1163.	0.2	31
31	Conformational Change and Ligand Binding in the Aristolochene Synthase Catalytic Cycle. Biochemistry, 2013, 52, 8094-8105.	1.2	30
32	Substrate polarization in enzyme catalysis: QM/MM analysis of the effect of oxaloacetate polarization on acetylâ€CoA enolization in citrate synthase. Proteins: Structure, Function and Bioinformatics, 2007, 69, 521-535.	1.5	29
33	A Multiscale Simulation Approach to Modeling Drugâ€“Protein Binding Kinetics. Journal of Chemical Theory and Computation, 2018, 14, 6093-6101.	2.3	29
34	Unpicking the Cause of Stereoselectivity in Actinorhodin Ketoreductase Variants with Atomistic Simulations. ACS Catalysis, 2019, 9, 2381-2394.	5.5	28
35	Molecular Dynamics as an Approach to Study Prion Protein Misfolding and the Effect of Pathogenic Mutations. Topics in Current Chemistry, 2011, 305, 169-197.	4.0	24
36	Structure and Function in Homodimeric Enzymes: Simulations of Cooperative and Independent Functional Motions. PLoS ONE, 2015, 10, e0133372.	1.1	24

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37	Ab initio QM/MM modelling of acetyl-CoA deprotonation in the enzyme citrate synthase. Journal of Molecular Graphics and Modelling, 2007, 26, 676-690.	1.3	23
38	Affinity of Avr2 for tomato cysteine protease Rcr3 correlates with the Avr2â€triggered Cfâ€2â€mediated hypersensitive response. Molecular Plant Pathology, 2011, 12, 21-30.	2.0	23
39	Visualizing the protons in a metalloenzyme electron proton transfer pathway. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 6484-6490.	3.3	22
40	Multiscale analysis of enantioselectivity in enzyme-catalysed â€˜lethal synthesisâ€™ using projector-based embedding. Royal Society Open Science, 2018, 5, 171390.	1.1	21
41	A Rieske oxygenase/epoxide hydrolase-catalysed reaction cascade creates oxygen heterocycles in mupirocin biosynthesis. Nature Catalysis, 2018, 1, 968-976.	16.1	21
42	Understanding Complex Mechanisms of Enzyme Reactivity: The Case of Limonene-1,2-Epoxide Hydrolases. ACS Catalysis, 2018, 8, 5698-5707.	5.5	20
43	Conformation control of the histidine kinase BceS of Bacillus subtilis by its cognate ABCâ€transporter facilitates needâ€based activation of antibiotic resistance. Molecular Microbiology, 2021, 115, 157-174.	1.2	20
44	Sensing Enzyme Activation Heat Capacity at the Single-Molecule Level Using Gold-Nanorod-Based Optical Whispering Gallery Modes. ACS Applied Nano Materials, 2021, 4, 4576-4583.	2.4	20
45	QM/MM simulations identify the determinants of catalytic activity differences between type II dehydroquinase enzymes. Organic and Biomolecular Chemistry, 2018, 16, 4443-4455.	1.5	19
46	Small Changes in Hydration Determine Cephalosporinase Activity of OXA-48 Î²-Lactamases. ACS Catalysis, 2020, 10, 6188-6196.	5.5	19
47	Cryptic Î²-Lactamase Evolution Is Driven by Low Î²-Lactam Concentrations. MSphere, 2021, 6, .	1.3	19
48	â€œLethal Synthesisâ€•of Fluorocitrate by Citrate Synthase Explained through QM/MM Modeling. Angewandte Chemie - International Edition, 2011, 50, 10349-10351.	7.2	18
49	Multiscale Simulations of Clavulanate Inhibition Identify the Reactive Complex in Class A Î²-Lactamases and Predict the Efficiency of Inhibition. Biochemistry, 2018, 57, 3560-3563.	1.2	17
50	The predominance of nucleotidyl activation in bacterial phosphonate biosynthesis. Nature Communications, 2019, 10, 3698.	5.8	16
51	An Efficient Computational Assay for Î²-Lactam Antibiotic Breakdown by Class A Î²-Lactamases. Journal of Chemical Information and Modeling, 2019, 59, 3365-3369.	2.5	16
52	Visualizing proteinâ€“ligand binding with chemical energy-wise decomposition (CHEWD): application to ligand binding in the kallikrein-8 S1 Site. Journal of Computer-Aided Molecular Design, 2019, 33, 461-475.	1.3	16
53	Mitochondrial import, health and mtDNA copy number variability using type II and type V CRISPR effectors. Journal of Cell Science, 2020, 133, .	1.2	16
54	Antimicrobial Resistance Conferred by OXA-48 Î²-Lactamases: Towards a Detailed Mechanistic Understanding. Antimicrobial Agents and Chemotherapy, 2021, 65, .	1.4	15

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55	Rigidifying a De Novo Enzyme Increases Activity and Induces a Negative Activation Heat Capacity. ACS Catalysis, 2021, 11, 11532-11541.	5.5	15
56	Identification of the quinolinedione inhibitor binding site in Cdc25 phosphatase B through docking and molecular dynamics simulations. Journal of Computer-Aided Molecular Design, 2017, 31, 995-1007.	1.3	13
57	Uncovering the Relationship between the Change in Heat Capacity for Enzyme Catalysis and Vibrational Frequency through Isotope Effect Studies. ACS Catalysis, 2018, 8, 5340-5349.	5.5	13
58	Taming the Reactivity of Monoterpene Synthases To Guide Regioselective Product Hydroxylation. ChemBioChem, 2020, 21, 985-990.	1.3	13
59	Enlighten2: molecular dynamics simulations of proteinâ€“ligand systems made accessible. Bioinformatics, 2020, 36, 5104-5106.	1.8	13
60	Redesigning the Molecular Choreography to Prevent Hydroxylation in Germacradien-11-ol Synthase Catalysis. ACS Catalysis, 2021, 11, 1033-1041.	5.5	13
61	An Esteraseâ€like Lyase Catalyzes Acetate Elimination in Spirotetronate/Spirotetramate Biosynthesis. Angewandte Chemie - International Edition, 2019, 58, 2305-2309.	7.2	12
62	Exposing the Interplay Between Enzyme Turnover, Protein Dynamics, and the Membrane Environment in Monoamine Oxidase B. Biochemistry, 2019, 58, 2362-2372.	1.2	12
63	Benchmarking quantum mechanical methods for calculating reaction energies of reactions catalyzed by enzymes. PeerJ Physical Chemistry, 0, 2, e8.	0.0	12
64	Quantum Mechanics/Molecular Mechanics Simulations Identify the Ring-Opening Mechanism of Creatininase. Biochemistry, 2017, 56, 6377-6388.	1.2	11
65	Catalytic mechanism of the colistin resistance protein MCR-1. Organic and Biomolecular Chemistry, 2021, 19, 3813-3819.	1.5	11
66	Simulations of membraneâ€bound diglycosylated human prion protein reveal potential protective mechanisms against misfolding. Journal of Neurochemistry, 2017, 142, 171-182.	2.1	10
67	How Static Disorder Mimics Decoherence in Anisotropy Pumpâ€“Probe Experiments on Purple-Bacteria Light Harvesting Complexes. Journal of Physical Chemistry B, 2016, 120, 11449-11463.	1.2	9
68	Rapid Estimation of Catalytic Efficiency by Cumulative Atomic Multipole Moments: Application to Ketosteroid Isomerase Mutants. Journal of Chemical Theory and Computation, 2017, 13, 945-955.	2.3	9
69	Molecular Rules Underpinning Enhanced Affinity Binding of Human T Cell Receptors Engineered for Immunotherapy. Molecular Therapy - Oncolytics, 2020, 18, 443-456.	2.0	9
70	Multiscale Simulations Identify Origins of Differential Carbapenem Hydrolysis by the OXA-48 Î²-Lactamase. ACS Catalysis, 2022, 12, 4534-4544.	5.5	9
71	Crystal structure of the putative cyclase IdmH from the indanomycin nonribosomal peptide synthase/polyketide synthase. IUCrJ, 2019, 6, 1120-1133.	1.0	8
72	Reliable In Silico Ranking of Engineered Therapeutic TCR Binding Affinities with MMPB/GBSA. Journal of Chemical Information and Modeling, 2022, 62, 577-590.	2.5	8

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73	Enzymatic synthesis of natural (+)-aristolochene from a non-natural substrate. Chemical Communications, 2016, 52, 14027-14030.	2.2	6
74	Peptide cargo tunes a network of correlated motions in human leucocyte antigens. FEBS Journal, 2020, 287, 3777-3793.	2.2	6
75	Chemical Mapping Exposes the Importance of Active Site Interactions in Governing the Temperature Dependence of Enzyme Turnover. ACS Catalysis, 2021, 11, 14854-14863.	5.5	6
76	Molecular Determinants of Carbocation Cyclisation in Bacterial Monoterpene Synthases. ChemBioChem, 2022, 23, .	1.3	5
77	Dynameomics: protein dynamics and unfolding across fold space. Biomolecular Concepts, 2010, 1, 335-344.	1.0	1
78	Multiâ€scale simulation reveals that an amino acid substitution increases photosensitizing reaction inputs in Rhodopsins. Journal of Computational Chemistry, 2020, 41, 2278-2295.	1.5	1
79	Path to Actinorhodin: Regio- and Stereoselective Ketone Reduction by a Type II Polyketide Ketoreductase Revealed in Atomistic Detail. Jacs Au, 2022, 2, 972-984.	3.6	1