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	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
2	Molecular Determinants of Carbocation Cyclisation in Bacterial Monoterpene Synthases. ChemBioChem, 2022, 23, .	1.3	5
3	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
4	Multiscale Simulations Identify Origins of Differential Carbapenem Hydrolysis by the OXA-48 Î²-Lactamase. ACS Catalysis, 2022, 12, 4534-4544.	5.5	9
5	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
6	Catalytic mechanism of the colistin resistance protein MCR-1. Organic and Biomolecular Chemistry, 2021, 19, 3813-3819.	1.5	11
7	Redesigning the Molecular Choreography to Prevent Hydroxylation in Germacradien-11-ol Synthase Catalysis. ACS Catalysis, 2021, 11, 1033-1041.	5.5	13
8	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
9	Loop Dynamics and Enzyme Catalysis in Protein Tyrosine Phosphatases. Journal of the American Chemical Society, 2021, 143, 3830-3845.	6.6	42
10	Cryptic Î²-Lactamase Evolution Is Driven by Low Î²-Lactam Concentrations. MSphere, 2021, 6, .	1.3	19
11	Antimicrobial Resistance Conferred by OXA-48 Î²-Lactamases: Towards a Detailed Mechanistic Understanding. Antimicrobial Agents and Chemotherapy, 2021, 65, .	1.4	15
12	Evolution of dynamical networks enhances catalysis in a designer enzyme. Nature Chemistry, 2021, 13, 1017-1022.	6.6	60
13	Rigidifying a De Novo Enzyme Increases Activity and Induces a Negative Activation Heat Capacity. ACS Catalysis, 2021, 11, 11532-11541.	5.5	15
14	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
15	Taming the Reactivity of Monoterpene Synthases To Guide Regioselective Product Hydroxylation. ChemBioChem, 2020, 21, 985-990.	1.3	13
16	Molecular Rules Underpinning Enhanced Affinity Binding of Human T Cell Receptors Engineered for Immunotherapy. Molecular Therapy - Oncolytics, 2020, 18, 443-456.	2.0	9
17	Enlighten2: molecular dynamics simulations of proteinâ€“ligand systems made accessible. Bioinformatics, 2020, 36, 5104-5106.	1.8	13
18	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

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19	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
20	Small Changes in Hydration Determine Cephalosporinase Activity of OXA-48 Î²-Lactamases. ACS Catalysis, 2020, 10, 6188-6196.	5.5	19
21	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
22	Peptide cargo tunes a network of correlated motions in human leucocyte antigens. FEBS Journal, 2020, 287, 3777-3793.	2.2	6
23	Enzyme evolution and the temperature dependence of enzyme catalysis. Current Opinion in Structural Biology, 2020, 65, 96-101.	2.6	54
24	Specificity of bispecific T cell receptors and antibodies targeting peptide-HLA. Journal of Clinical Investigation, 2020, 130, 2673-2688.	3.9	50
25	The predominance of nucleotidyl activation in bacterial phosphonate biosynthesis. Nature Communications, 2019, 10, 3698.	5.8	16
26	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
27	An Esteraseâ€like Lyase Catalyzes Acetate Elimination in Spirotetronate/Spirotetramate Biosynthesis. Angewandte Chemie - International Edition, 2019, 58, 2305-2309.	7.2	12
28	Unpicking the Cause of Stereoselectivity in Actinorhodin Ketoreductase Variants with Atomistic Simulations. ACS Catalysis, 2019, 9, 2381-2394.	5.5	28
29	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
30	Exposing the Interplay Between Enzyme Turnover, Protein Dynamics, and the Membrane Environment in Monoamine Oxidase B. Biochemistry, 2019, 58, 2362-2372.	1.2	12
31	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1393.	6.2	110
32	Crystal structure of the putative cyclase IdmH from the indanomycin nonribosomal peptide synthase/polyketide synthase. IUCrJ, 2019, 6, 1120-1133.	1.0	8
33	Multiscale analysis of enantioselectivity in enzyme-catalysed â€˜lethal synthesisâ€™ using projector-based embedding. Royal Society Open Science, 2018, 5, 171390.	1.1	21
34	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
35	Dynamical origins of heat capacity changes in enzyme-catalysed reactions. Nature Communications, 2018, 9, 1177.	5.8	64
36	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

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37	A Rieske oxygenase/epoxide hydrolase-catalysed reaction cascade creates oxygen heterocycles in mupirocin biosynthesis. Nature Catalysis, 2018, 1, 968-976.	16.1	21
38	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
39	A Multiscale Simulation Approach to Modeling Drugâ€“Protein Binding Kinetics. Journal of Chemical Theory and Computation, 2018, 14, 6093-6101.	2.3	29
40	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
41	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
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	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
44	Simulations of membraneâ€bound diglycosylated human prion protein reveal potential protective mechanisms against misfolding. Journal of Neurochemistry, 2017, 142, 171-182.	2.1	10
45	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
46	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
47	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
48	Quantum Mechanics/Molecular Mechanics Simulations Identify the Ring-Opening Mechanism of Creatininase. Biochemistry, 2017, 56, 6377-6388.	1.2	11
49	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
50	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
51	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
52	Enzymatic synthesis of natural (+)-aristolochene from a non-natural substrate. Chemical Communications, 2016, 52, 14027-14030.	2.2	6
53	On the Temperature Dependence of Enzyme-Catalyzed Rates. Biochemistry, 2016, 55, 1681-1688.	1.2	233
54	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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55	Structural and Dynamic Properties of the Human Prion Protein. Biophysical Journal, 2014, 106, 1152-1163.	0.2	31
56	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
57	QM/MM simulations as an assay for carbapenemase activity in class A Î²-lactamases. Chemical Communications, 2014, 50, 14736-14739.	2.2	43
58	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
59	Conformational Change and Ligand Binding in the Aristolochene Synthase Catalytic Cycle. Biochemistry, 2013, 52, 8094-8105.	1.2	30
60	Combined Quantum Mechanics/Molecular Mechanics (QM/MM) Methods in Computational Enzymology. Biochemistry, 2013, 52, 2708-2728.	1.2	471
61	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
62	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
63	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
64	â€œLethal Synthesisâ€•of Fluorocitrate by Citrate Synthase Explained through QM/MM Modeling. Angewandte Chemie - International Edition, 2011, 50, 10349-10351.	7.2	18
65	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
66	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
67	Dynameomics: A Comprehensive Database of Protein Dynamics. Structure, 2010, 18, 423-435.	1.6	131
68	Influence of pH on the Human Prion Protein: Insights into the Early Steps ofÂMisfolding. Biophysical Journal, 2010, 99, 2289-2298.	0.2	75
69	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
70	Dynameomics: protein dynamics and unfolding across fold space. Biomolecular Concepts, 2010, 1, 335-344.	1.0	1
71	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
72	The consequences of pathogenic mutations to the human prion protein. Protein Engineering, Design and Selection, 2009, 22, 461-468.	1.0	73

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73	Computational enzymology: insight into biological catalysts from modelling. Natural Product Reports, 2008, 25, 1001.	5.2	51
74	Biomolecular simulation and modelling: status, progress and prospects. Journal of the Royal Society Interface, 2008, 5, 173-190.	1.5	77
75	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
76	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
77	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
78	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
79	Benchmarking quantum mechanical methods for calculating reaction energies of reactions catalyzed by enzymes. PeerJ Physical Chemistry, 0, 2, e8.	0.0	12