Adrian J Mulholland

List of Publications by Year
in descending order

245	12,022	20797 60	42364 92
papers	citations	h-index	g-index

314	314	314	9872
all docs	docs citations	times ranked	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	Free fatty acid binding pocket in the locked structure of SARS-CoV-2 spike protein. Science, 2020, 370, 725-730.	6.0	348
3	Atomic Description of an Enzyme Reaction Dominated by Proton Tunneling. Science, 2006, 312, 237-241.	6.0	304
4	High-Accuracy Computation of Reaction Barriers in Enzymes. Angewandte Chemie - International Edition, 2006, 45, 6856-6859.	7.2	253
5	On the Temperature Dependence of Enzyme-Catalyzed Rates. Biochemistry, 2016, 55, 1681-1688.	1.2	233
6	Taking Ockham's razor to enzyme dynamics and catalysis. Nature Chemistry, 2012, 4, 169-176.	6.6	217
7	Does Compound I Vary Significantly between Isoforms of Cytochrome P450?. Journal of the American Chemical Society, 2011, 133, 15464-15474.	6.6	188
8	Modelling enzyme reaction mechanisms, specificity and catalysis. Drug Discovery Today, 2005, 10, 1393-1402.	3.2	169
9	Insights into Chorismate Mutase Catalysis from a Combined QM/MM Simulation of the Enzyme Reaction. Journal of the American Chemical Society, 1995, 117, 11345-11350.	6.6	157
10	Electronic Structure of Compound I in Human Isoforms of Cytochrome P450 from QM/MM Modeling. Journal of the American Chemical Society, 2005, 127, 12900-12908.	6.6	157
11	A practical guide to modelling enzyme-catalysed reactions. Chemical Society Reviews, 2012, 41, 3025.	18.7	156
12	Inclusion of Dispersion Effects Significantly Improves Accuracy of Calculated Reaction Barriers for Cytochrome P450 Catalyzed Reactions. Journal of Physical Chemistry Letters, 2010, 1, 3232-3237.	2.1	153
13	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
14	Aromatic Hydroxylation by Cytochrome P450:Â Model Calculations of Mechanism and Substituent Effects. Journal of the American Chemical Society, 2003, 125, 15004-15005.	6.6	135
15	Mechanisms of Antibiotic Resistance:Â QM/MM Modeling of the Acylation Reaction of a Class A Î²-Lactamase with Benzylpenicillin. Journal of the American Chemical Society, 2005, 127, 4454-4465.	6.6	133
16	Mechanism and structureâ€“reactivity relationships for aromatic hydroxylation by cytochrome P450. Organic and Biomolecular Chemistry, 2004, 2, 2998-3005.	1.5	130
17	P450-Catalyzed Regio- and Diastereoselective Steroid Hydroxylation: Efficient Directed Evolution Enabled by Mutability Landscaping. ACS Catalysis, 2018, 8, 3395-3410.	5.5	128
18	Ab Initio QM/MM Study of the Citrate Synthase Mechanism. A Low-Barrier Hydrogen Bond Is not Involved. Journal of the American Chemical Society, 2000, 122, 534-535.	6.6	122

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19	Unraveling the role of protein dynamics in dihydrofolate reductase catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 16344-16349.	3.3	119
20	Multiscale methods in drug design bridge chemical and biological complexity in the search for cures. Nature Reviews Chemistry, 2018, 2, .	13.8	112
21	Quantum Mechanics/Molecular Mechanics Modeling of Regioselectivity of Drug Metabolism in Cytochrome P450 2C9. Journal of the American Chemical Society, 2013, 135, 8001-8015.	6.6	110
22	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1393.	6.2	110
23	Investigations of enzyme-catalysed reactions with combined quantum mechanics/molecular mechanics (QM/MM) methods. International Reviews in Physical Chemistry, 2010, 29, 65-133.	0.9	109
24	Compound I Reactivity Defines Alkene Oxidation Selectivity in Cytochrome P450cam. Journal of Physical Chemistry B, 2010, 114, 1156-1162.	1.2	108
25	QM/MM Modeling of Benzene Hydroxylation in Human Cytochrome P450 2C9. Journal of Physical Chemistry A, 2008, 112, 13149-13156.	1.1	107
26	Insights into the Mechanistic Basis of Plasmid-Mediated Colistin Resistance from Crystal Structures of the Catalytic Domain of MCR-1. Scientific Reports, 2017, 7, 39392.	1.6	107
27	Differential Transition-State Stabilization in Enzyme Catalysis:Â Quantum Chemical Analysis of Interactions in the Chorismate Mutase Reaction and Prediction of the Optimal Catalytic Field. Journal of the American Chemical Society, 2004, 126, 16148-16159.	6.6	104
28	Computational enzymology. Chemical Communications, 2010, 46, 2354.	2.2	104
29	Transition state stabilization and substrate strain in enzyme catalysis: ab initio QM/MM modelling of the chorismate mutase reaction. Organic and Biomolecular Chemistry, 2004, 2, 968.	1.5	98
30	Understanding the determinants of selectivity in drug metabolism through modeling of dextromethorphan oxidation by cytochrome P450. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6050-6055.	3.3	98
31	Acetyl-CoA enolization in citrate synthase: A quantum mechanical/molecular mechanical (QM/MM) study. Proteins: Structure, Function and Bioinformatics, 1997, 27, 9-25.	1.5	96
32	Teaching Enzyme Catalysis Using Interactive Molecular Dynamics in Virtual Reality. Journal of Chemical Education, 2019, 96, 2488-2496.	1.1	92
33	A Quantum Mechanical/Molecular Mechanical Study of the Hydroxylation of Phenol and Halogenated Derivatives by Phenol Hydroxylase. Journal of the American Chemical Society, 2000, 122, 8728-8738.	6.6	91
34	Construction and in vivo assembly of a catalytically proficient and hyperthermostable de novo enzyme. Nature Communications, 2017, 8, 358.	5.8	91
35	Quantum Mechanical/Molecular Mechanical Free Energy Simulations of the GlutathioneS-Transferase (M1-1) Reaction with Phenanthrene 9,10-Oxide. Journal of the American Chemical Society, 2002, 124, 9926-9936.	6.6	90
36	An efficient method for the calculation of quantum mechanics/molecular mechanics free energies. Journal of Chemical Physics, 2008, 128, 014109.	1.2	89

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37	Sampling molecular conformations and dynamics in a multiuser virtual reality framework. Science Advances, 2018, 4, eaat2731.	4.7	88
38	Mechanism of inhibition of SARS-CoV-2 M‹sup›pro‹/sup› by N3 peptidyl Michael acceptor explained by QM/MM simulations and design of new derivatives with tunable chemical reactivity. Chemical Science, 2021, 12, 1433-1444.	3.7	87
39	Multiple high-level QM/MM reaction paths demonstrate transition-state stabilization in chorismate mutase: correlation of barrier height with transition-state stabilization. Chemical Communications, 2005, , 5068.	2.2	85
40	Effects of Dispersion in Density Functional Based Quantum Mechanical/Molecular Mechanical Calculations on Cytochrome P450 Catalyzed Reactions. Journal of Chemical Theory and Computation, 2012, 8, 4637-4645.	2.3	85
41	Conformational Effects in Enzyme Catalysis: Reaction via a High Energy Conformation in Fatty Acid Amide Hydrolase. Biophysical Journal, 2007, 92, L20-L22.	0.2	77
42	Biomolecular simulation and modelling: status, progress and prospects. Journal of the Royal Society Interface, 2008, 5, 173-190.	1.5	77
43	Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARSâ€CoVâ€2 Spike Protein**. Angewandte Chemie - International Edition, 2021, 60, 7098-7110.	7.2	77
44	Ab Initio QM/MM Modeling of the Hydroxylation Step in p-Hydroxybenzoate Hydroxylase. Journal of Physical Chemistry B, 2003, 107, 2118-2126.	1.2	76
45	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
46	Protein dynamics and enzyme catalysis: Insights from simulations. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 1077-1092.	1.1	74
47	Temperature, Dynamics, and Enzyme-Catalyzed Reaction Rates. Annual Review of Biophysics, 2020, 49, 163-180.	4.5	74
48	Insights into enzyme catalysis from QM/MM modelling: transition state stabilization in chorismate mutase. Molecular Physics, 2003, 101, 2695-2714.	0.8	73
49	Molecular mechanisms of antibiotic resistance: QM/MM modelling of deacylation in a class A Î²-lactamase. Organic and Biomolecular Chemistry, 2006, 4, 206-210.	1.5	73
50	A water-swap reaction coordinate for the calculation of absolute proteinâ€“ligand binding free energies. Journal of Chemical Physics, 2011, 134, 054114.	1.2	73
51	Rapid decomposition and visualisation of proteinâ€“ligand binding free energies by residue and by water. Faraday Discussions, 2014, 169, 477-499.	1.6	71
52	Interactive molecular dynamics in virtual reality from quantum chemistry to drug binding: An open-source multi-person framework. Journal of Chemical Physics, 2019, 150, 220901.	1.2	69
53	Identification of Glu166 as the General Base in the Acylation Reaction of Class A Î²-Lactamases through QM/MM Modeling. Journal of the American Chemical Society, 2003, 125, 9590-9591.	6.6	68
54	QM/MM simulations predict a covalent intermediate in the hen egg white lysozyme reaction with its natural substrate. Chemical Communications, 2008, , 4425.	2.2	66

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55	Analysis of chorismate mutase catalysis by QM/MM modelling of enzyme-catalysed and uncatalysed reactions. Organic and Biomolecular Chemistry, 2011, 9, 1578.	1.5	66
56	IMPRESSION â€“ prediction of NMR parameters for 3-dimensional chemical structures using machine learning with near quantum chemical accuracy. Chemical Science, 2020, 11, 508-515.	3.7	66
57	Computer modelling of enzyme catalysed reaction mechanisms. Protein Engineering, Design and Selection, 1993, 6, 133-147.	1.0	65
58	Identification of productive inhibitor binding orientation in fatty acid amide hydrolase (FAAH) by QM/MM mechanistic modelling. Chemical Communications, 2008, , 214-216.	2.2	65
59	Dynamical origins of heat capacity changes in enzyme-catalysed reactions. Nature Communications, 2018, 9, 1177.	5.8	64
60	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
61	Correlation of Calculated Activation Energies with Experimental Rate Constants for an Enzyme Catalyzed Aromatic Hydroxylation. Journal of the American Chemical Society, 1998, 120, 7641-7642.	6.6	62
62	QM/MM modelling of oleamide hydrolysis in fatty acid amide hydrolase (FAAH) reveals a new mechanism of nucleophile activation. Chemical Communications, 2005, , 4399.	2.2	62
63	QM/MM modeling of compound I active species in cytochrome P450, cytochrome C peroxidase, and ascorbate peroxidase. Journal of Computational Chemistry, 2006, 27, 1352-1362.	1.5	62
64	Structural Fluctuations in Enzyme-Catalyzed Reactions: Determinants of Reactivity in Fatty Acid Amide Hydrolase from Multivariate Statistical Analysis of Quantum Mechanics/Molecular Mechanics Paths. Journal of Chemical Theory and Computation, 2010, 6, 2948-2960.	2.3	61
65	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
66	De Novo-Designed Î±-Helical Barrels as Receptors for Small Molecules. ACS Synthetic Biology, 2018, 7, 1808-1816.	1.9	60
67	Evolution of dynamical networks enhances catalysis in a designer enzyme. Nature Chemistry, 2021, 13, 1017-1022.	6.6	60
68	Hydrogen tunnelling in enzyme-catalysed H-transfer reactions: flavoprotein and quinoprotein systems. Philosophical Transactions of the Royal Society B: Biological Sciences, 2006, 361, 1375-1386.	1.8	59
69	Constructing ion channels from water-soluble Î±-helical barrels. Nature Chemistry, 2021, 13, 643-650.	6.6	59
70	Quantum Mechanics/Molecular Mechanics Modeling of Substrate-Assisted Catalysis in Family 18 Chitinases: Conformational Changes and the Role of Asp142 in Catalysis in ChiB. Biochemistry, 2011, 50, 4697-4711.	1.2	58
71	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
72	Conformational effects in enzyme catalysis: QM/MM free energy calculation of the â€˜NACâ€™ contribution in chorismate mutase. Chemical Communications, 2004, , 1238-1239.	2.2	57

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73	A Community Letter Regarding Sharing Biomolecular Simulation Data for COVID-19. Journal of Chemical Information and Modeling, 2020, 60, 2653-2656.	2.5	57
74	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
75	Determinants of Reactivity and Selectivity in Soluble Epoxide Hydrolase from Quantum Mechanics/Molecular Mechanics Modeling. Biochemistry, 2012, 51, 1774-1786.	1.2	55
76	Enzyme evolution and the temperature dependence of enzyme catalysis. Current Opinion in Structural Biology, 2020, 65, 96-101.	2.6	54
77	Discovery of SARS-CoV-2 M^{pro} peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	3.7	54
78	Tunneling and Classical Paths for Proton Transfer in an Enzyme Reaction Dominated by Tunneling:Â Oxidation of Tryptamine by Aromatic Amine Dehydrogenase. Journal of Physical Chemistry B, 2007, 111, 3032-3047.	1.2	53
79	Chemical accuracy in QM/MM calculations on enzyme-catalysed reactions. Chemistry Central Journal, 2007, 1, 19.	2.6	53
80	Computational enzymology: insight into biological catalysts from modelling. Natural Product Reports, 2008, 25, 1001.	5.2	51
81	A Photoresponsive Stiffâ€Stilbene Ligand Fuels the Reversible Unfolding of Gâ€Quadruplex DNA. Angewandte Chemie - International Edition, 2019, 58, 4334-4338.	7.2	50
82	Analysis of polarization in QM/MM modelling of biologically relevant hydrogen bonds. Journal of the Royal Society Interface, 2008, 5, 207-216.	1.5	49
83	Large-Scale Density Functional Theory Transition State Searching in Enzymes. Journal of Physical Chemistry Letters, 2014, 5, 3614-3619.	2.1	49
84	Designing better enzymes: Insights from directed evolution. Current Opinion in Structural Biology, 2021, 67, 212-218.	2.6	49
85	Modeling Biotransformation Reactions by Combined Quantum Mechanical / Molecular Mechanical Approaches: From Structure to Activity. Current Topics in Medicinal Chemistry, 2003, 3, 1241-1256.	1.0	49
86	Compatibility of Quantum Chemical Methods and Empirical (MM) Water Models in Quantum Mechanics/Molecular Mechanics Liquid Water Simulations. Journal of Physical Chemistry Letters, 2010, 1, 219-223.	2.1	47
87	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
88	Maintaining and breaking symmetry in homomeric coiled-coil assemblies. Nature Communications, 2018, 9, 4132.	5.8	45
89	Molecular Basis of Class A Î²-Lactamase Inhibition by Relebactam. Antimicrobial Agents and Chemotherapy, 2019, 63, .	1.4	45
90	Computational enzymology: modelling the mechanisms of biological catalysts. Biochemical Society Transactions, 2008, 36, 22-26.	1.6	44

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91	Allosteric communication in class A Î²-lactamases occurs via cooperative coupling of loop dynamics. ELife, 2021, 10, .	2.8	44
92	Combined Quantum and Molecular Mechanical Study of DNA Crosslinking by Nitrous Acid. Journal of the American Chemical Society, 1995, 117, 4706-4707.	6.6	43
93	QM/MM simulations as an assay for carbapenemase activity in class A Î²-lactamases. Chemical Communications, 2014, 50, 14736-14739.	2.2	43
94	A potential interaction between the SARS-CoV-2 spike protein and nicotinic acetylcholine receptors. Biophysical Journal, 2021, 120, 983-993.	0.2	43
95	Mechanisms of reaction in cytochrome P450: hydroxylation of camphor in P450cam. Organic and Biomolecular Chemistry, 2006, 4, 3931.	1.5	42
96	A Multiscale Approach to Modelling Drug Metabolism by Membrane-Bound Cytochrome P450 Enzymes. PLoS Computational Biology, 2014, 10, e1003714.	1.5	42
97	Emergence of a Negative Activation Heat Capacity during Evolution of a Designed Enzyme. Journal of the American Chemical Society, 2019, 141, 11745-11748.	6.6	42
98	Molecular Determinants of Xenobiotic Metabolism:â€‰ QM/MM Simulation of the Conversion of 1-Chloro-2,4-dinitrobenzene Catalyzed by M1-1 Glutathione S-Transferase. Biochemistry, 2007, 46, 6353-6363.	1.2	41
99	Analysis of Classical and Quantum Paths for Deprotonation of Methylamine by Methylamine Dehydrogenase. ChemPhysChem, 2007, 8, 1816-1835.	1.0	41
100	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
101	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
102	High Level QM/MM Modeling of the Formation of the Tetrahedral Intermediate in the Acylation of Wild Type and K73A Mutant TEM-1 Class A Î²-Lactamase. Journal of Physical Chemistry A, 2009, 113, 11984-11994.	1.1	38
103	Long Time Scale GPU Dynamics Reveal the Mechanism of Drug Resistance of the Dual Mutant I223R/H275Y Neuraminidase from H1N1-2009 Influenza Virus. Biochemistry, 2012, 51, 4364-4375.	1.2	37
104	QM/MM Free-Energy Simulations of Reaction in Serratia marcescens Chitinase B Reveal the Protonation State of Asp142 and the Critical Role of Tyr214. Journal of Physical Chemistry B, 2014, 118, 4771-4783.	1.2	37
105	The Fe-CO Bond Energy in Myoglobin: A QM/MM Study of the Effect of Tertiary Structure. Biophysical Journal, 2006, 90, L27-L29.	0.2	36
106	Insights into the mechanism and inhibition of fatty acid amide hydrolase from quantum mechanics/molecular mechanics (QM/MM) modelling. Biochemical Society Transactions, 2009, 37, 363-367.	1.6	36
107	The calculation of product quantum state distributions and partial cross-sections in time-dependent molecular collision and photodissociation theory. Computer Physics Communications, 1991, 63, 126-134.	3.0	35
108	Combined quantum mechanical and molecular mechanical reaction pathway calculation for aromatic hydroxylation by p-hydroxybenzoate-3-hydroxylase. Journal of Molecular Graphics and Modelling, 1999, 17, 163-175.	1.3	35

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109	Quantum Mechanics/Molecular Mechanics Modeling of Fatty Acid Amide Hydrolase Reactivation Distinguishes Substrate from Irreversible Covalent Inhibitors. Journal of Medicinal Chemistry, 2013, 56, 2500-2512.	2.9	35
110	Computational Assay of H7N9 Influenza Neuraminidase Reveals R292K Mutation Reduces Drug Binding Affinity. Scientific Reports, 2013, 3, 3561.	1.6	35
111	Modeling Enzyme Reaction Intermediates and Transition States:Â Citrate Synthase. Journal of Physical Chemistry B, 1998, 102, 6635-6646.	1.2	34
112	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
113	Discovery of New and Potent InhA Inhibitors as Antituberculosis Agents: Structure-Based Virtual Screening Validated by Biological Assays and X-ray Crystallography. Journal of Chemical Information and Modeling, 2020, 60, 226-234.	2.5	34
114	Biocatalytic Routes to Lactone Monomers for Polymer Production. Biochemistry, 2018, 57, 1997-2008.	1.2	33
115	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
116	Active site dynamics and combined quantum mechanics/molecular mechanics (QM/MM) modelling of a HIV-1 reverse transcriptase/DNA/dTTP complex. Journal of Molecular Graphics and Modelling, 2007, 26, 1-13.	1.3	32
117	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
118	Unlocking Nicotinic Selectivity via Direct Câ€'H Functionalization of (âˆ')-Cytisine. CheM, 2018, 4, 1710-1725.	5.8	31
119	QM/MM studies of the electronic structure of the compound I intermediate in cytochrome c peroxidase and ascorbate peroxidase. Dalton Transactions, 2005, , 3470.	1.6	30
120	Computational and experimental studies on the catalytic mechanism of biliverdin-IXÎ² reductase. Biochemical Journal, 2008, 411, 475-484.	1.7	30
121	Conformational Change and Ligand Binding in the Aristolochene Synthase Catalytic Cycle. Biochemistry, 2013, 52, 8094-8105.	1.2	30
122	Elucidation of Nonadditive Effects in Proteinâ€"Ligand Binding Energies: Thrombin as a Case Study. Journal of Physical Chemistry B, 2016, 120, 5340-5350.	1.2	30
123	Mechanistic Insights into the Reaction of Chlorination of Tryptophan Catalyzed by Tryptophan 7-Halogenase. Scientific Reports, 2017, 7, 17395.	1.6	30
124	Interactive Molecular Dynamics in Virtual Reality Is an Effective Tool for Flexible Substrate and Inhibitor Docking to the SARS-CoV-2 Main Protease. Journal of Chemical Information and Modeling, 2020, 60, 5803-5814.	2.5	30
125	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
126	Understanding the role of carbamate reactivity in fatty acid amide hydrolase inhibition by QM/MM mechanistic modelling. Chemical Communications, 2011, 47, 2517.	2.2	29

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127	Mechanism of C-terminal intein cleavage in protein splicing from QM/MM molecular dynamics simulations. Organic and Biomolecular Chemistry, 2012, 10, 1207-1218.	1.5	29
128	A Multiscale Simulation Approach to Modeling Drugâ€“Protein Binding Kinetics. Journal of Chemical Theory and Computation, 2018, 14, 6093-6101.	2.3	29
129	Multiscale simulation approaches to modeling drugâ€“protein binding. Current Opinion in Structural Biology, 2020, 61, 213-221.	2.6	29
130	Visible-light photoswitching of ligand binding mode suggests G-quadruplex DNA as a target for photopharmacology. Chemical Communications, 2020, 56, 5186-5189.	2.2	29
131	The QM/MM Approach to Enzymatic Reactions. Theoretical and Computational Chemistry, 2001, , 597-653.	0.2	28
132	A catalytic role for methionine revealed by a combination of computation and experiments on phosphite dehydrogenase. Chemical Science, 2014, 5, 2191-2199.	3.7	28
133	Molecular dynamics simulations support the hypothesis that the brGDGT paleothermometer is based on homeoviscous adaptation. Geochimica Et Cosmochimica Acta, 2021, 312, 44-56.	1.6	28
134	Conformational Effects on the pro - S Hydrogen Abstraction Reaction in Cyclooxygenase-1: An Integrated QM/MM and MD Study. Biophysical Journal, 2013, 104, L5-L7.	0.2	27
135	Quantum Mechanics/Molecular Mechanics Modeling of Drug Metabolism: Mexiletine N-Hydroxylation by Cytochrome P450 1A2. Chemical Research in Toxicology, 2016, 29, 963-971.	1.7	27
136	Projector-Based Embedding Eliminates Density Functional Dependence for QM/MM Calculations of Reactions in Enzymes and Solution. Journal of Chemical Information and Modeling, 2019, 59, 2063-2078.	2.5	27
137	Natural variants modify Klebsiella pneumoniae carbapenemase (KPC) acylâ€“enzyme conformational dynamics to extend antibiotic resistance. Journal of Biological Chemistry, 2021, 296, 100126.	1.6	27
138	Cooperative symmetric to asymmetric conformational transition of the apoâ€form of scavenger decapping enzyme revealed by simulations. Proteins: Structure, Function and Bioinformatics, 2008, 70, 498-508.	1.5	26
139	Trends in predicted chemoselectivity of cytochrome P450 oxidation: B3LYP barrier heights for epoxidation and hydroxylation reactions. Journal of Molecular Graphics and Modelling, 2014, 52, 30-35.	1.3	26
140	Dissecting the low catalytic capability of flavin-dependent halogenases. Journal of Biological Chemistry, 2021, 296, 100068.	1.6	26
141	BioSimSpace: An interoperable Python framework for biomolecular simulation. Journal of Open Source Software, 2019, 4, 1831.	2.0	26
142	QM/MM study on the mechanism of peptide hydrolysis by carboxypeptidase A. Computational and Theoretical Chemistry, 2009, 898, 106-114.	1.5	25
143	Modeling Protein Splicing: Reaction Pathway for C-Terminal Splice and Intein Scission. Journal of Physical Chemistry B, 2009, 113, 5607-5616.	1.2	25
144	A General Mechanism for Signal Propagation in the Nicotinic Acetylcholine Receptor Family. Journal of the American Chemical Society, 2019, 141, 19953-19958.	6.6	25

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145	Biomolecular Simulations in the Time of COVID-19, and After. Computing in Science and Engineering, 2020, 22, 30-36.	1.2	25
146	Interactive molecular dynamics in virtual reality for accurate flexible protein-ligand docking. PLoS ONE, 2020, 15, e0228461.	1.1	25
147	Structure and Function in Homodimeric Enzymes: Simulations of Cooperative and Independent Functional Motions. PLoS ONE, 2015, 10, e0133372.	1.1	24
148	Combined Quantum Mechanics/Molecular Mechanics (QM/MM) Simulations for Proteinâ€“Ligand Complexes: Free Energies of Binding of Water Molecules in Influenza Neuraminidase. Journal of Physical Chemistry B, 2015, 119, 997-1001.	1.2	24
149	Identification of the Initial Steps in Signal Transduction in the Î±4Î²2 Nicotinic Receptor: Insights from Equilibrium and Nonequilibrium Simulations. Structure, 2019, 27, 1171-1183.e3.	1.6	24
150	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
151	Dynamical nonequilibrium molecular dynamics reveals the structural basis for allostery and signal propagation in biomolecular systems. European Physical Journal B, 2021, 94, 144.	0.6	23
152	Structural insights in cell-type specific evolution of intra-host diversity by SARS-CoV-2. Nature Communications, 2022, 13, 222.	5.8	23
153	MM and QM/MM Modeling of Threonyl-tRNA Synthetase: Model Testing and Simulations. Structural Chemistry, 2004, 15, 405-414.	1.0	22
154	Analysis and Assay of Oseltamivir-Resistant Mutants of Influenza Neuraminidase via Direct Observation of Drug Unbinding and Rebinding in Simulation. Biochemistry, 2013, 52, 8150-8164.	1.2	22
155	Role of Active Site Residues in Promoting Cobaltâ€“Carbon Bond Homolysis in Adenosylcobalamin-Dependent Mutases Revealed through Experiment and Computation. Biochemistry, 2014, 53, 169-177.	1.2	22
156	Quantum Mechanics/Molecular Mechanics (QM/MM) Calculations Support a Concerted Reaction Mechanism for the Zika Virus NS2B/NS3 Serine Protease with Its Substrate. Journal of Physical Chemistry B, 2019, 123, 2889-2903.	1.2	22
157	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
158	Mechanism of covalent binding of ibrutinib to Bruton's tyrosine kinase revealed by QM/MM calculations. Chemical Science, 2021, 12, 5511-5516.	3.7	22
159	QM/MM Modelling of Drug-Metabolizing Enzymes. Current Topics in Medicinal Chemistry, 2014, 14, 1339-1347.	1.0	22
160	Multiscale analysis of enantioselectivity in enzyme-catalysed â€˜lethal synthesisâ€™ using projector-based embedding. Royal Society Open Science, 2018, 5, 171390.	1.1	21
161	Mechanistic Insights into the Ligand-Induced Unfolding of an RNA G-Quadruplex. Journal of the American Chemical Society, 2022, 144, 935-950.	6.6	21
162	Quantum chemical analysis of reaction paths in chorismate mutase: Conformational effects and electrostatic stabilization. International Journal of Quantum Chemistry, 2007, 107, 2274-2285.	1.0	20

#	Article	IF	Citations
163	High-Level QM/MM Calculations Support the Concerted Mechanism for Michael Addition and Covalent Complex Formation in Thymidylate Synthase. Journal of Chemical Theory and Computation, 2015, 11, 713-722.	2.3	20
164	Structural Insights from Molecular Dynamics Simulations of Tryptophan 7-Halogenase and Tryptophan 5-Halogenase. ACS Omega, 2018, 3, 4847-4859.	1.6	20
165	Understanding Complex Mechanisms of Enzyme Reactivity: The Case of Limonene-1,2-Epoxide Hydrolases. ACS Catalysis, 2018, 8, 5698-5707.	5.5	20
166	Cyclic boronates as versatile scaffolds for KPC-2 Î²-lactamase inhibition. RSC Medicinal Chemistry, 2020, 11, 491-496.	1.7	20
167	Application of a SCC-DFTB QM/MM approach to the investigation of the catalytic mechanism of fatty acid amide hydrolase. Journal of Molecular Modeling, 2011, 17, 2375-2383.	0.8	19
168	Comparison of DFT and ab initio QM/MM methods for modelling reaction in chorismate synthase. Chemical Physics Letters, 2014, 608, 380-385.	1.2	19
169	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
170	Molecular Dynamics Simulation Framework to Probe the Binding Hypothesis of CYP3A4 Inhibitors. International Journal of Molecular Sciences, 2019, 20, 4468.	1.8	19
171	Small Changes in Hydration Determine Cephalosporinase Activity of OXA-48 Î²-Lactamases. ACS Catalysis, 2020, 10, 6188-6196.	5.5	19
172	The fatty acid site is coupled to functional motifs in the SARS-CoV-2 spike protein and modulates spike allosteric behaviour. Computational and Structural Biotechnology Journal, 2022, 20, 139-147.	1.9	19
173	â€œLethal Synthesisâ€•of Fluorocitrate by Citrate Synthase Explained through QM/MM Modeling. Angewandte Chemie - International Edition, 2011, 50, 10349-10351.	7.2	18
174	Protein dynamics and enzyme catalysis: the ghost in the machine?. Biochemical Society Transactions, 2012, 40, 515-521.	1.6	18
175	Lennardâ^'Jones Parameters for B3LYP/CHARMM27 QM/MM Modeling of Nucleic Acid Bases. Journal of Chemical Theory and Computation, 2009, 5, 396-410.	2.3	17
176	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
177	Impact of Warhead Modulations on the Covalent Inhibition of SARS-CoV-2 M^{pro} Explored by QM/MM Simulations. ACS Catalysis, 2022, 12, 698-708.	5.5	17
178	A model of the condensation step in the citrate synthase reaction. Computational and Theoretical Chemistry, 1998, 427, 175-184.	1.5	16
179	Enzyme dynamics and catalysis in the mechanism of DNA polymerase. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	16
180	Ab Initio QM/MM Modeling of the Rate-Limiting Proton Transfer Step in the Deamination of Tryptamine by Aromatic Amine Dehydrogenase. Journal of Physical Chemistry B, 2017, 121, 9785-9798.	1.2	16

#	Article	IF	Citations
181	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
182	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
183	Structural resolution of switchable states of a de novo peptide assembly. Nature Communications, 2021, 12, 1530.	5.8	16
184	Calculations on the substrates of citrate synthase I. Oxaloacetate. Computational and Theoretical Chemistry, 1998, 429, 13-21.	1.5	15
185	Computer simulations of quantum tunnelling in enzyme-catalysed hydrogen transfer reactions. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 78-97.	2.2	15
186	Limitations of Ligand-Only Approaches for Predicting the Reactivity of Covalent Inhibitors. Journal of Chemical Information and Modeling, 2019, 59, 4220-4227.	2.5	15
187	A Photoresponsive Stiffâ€Stilbene Ligand Fuels the Reversible Unfolding of Gâ€Quadruplex DNA. Angewandte Chemie, 2019, 131, 4378-4382.	1.6	15
188	Enhanced sampling molecular dynamics simulations correctly predict the diverse activities of a series of stiff-stilbene G-quadruplex DNA ligands. Chemical Science, 2021, 12, 1415-1426.	3.7	15
189	Rigidifying a De Novo Enzyme Increases Activity and Induces a Negative Activation Heat Capacity. ACS Catalysis, 2021, 11, 11532-11541.	5.5	15
190	A comparison of semiempirical and ab initio transition states for HF elimination in unimolecular decompositions. International Journal of Quantum Chemistry, 1994, 51, 161-172.	1.0	14
191	QM and QM/MM studies of selectivity in organic and bioorganic chemistry. Journal of Physical Organic Chemistry, 2006, 19, 608-615.	0.9	14
192	A robust and stereocomplementary panel of ene-reductase variants for gram-scale asymmetric hydrogenation. Molecular Catalysis, 2021, 502, 111404.	1.0	14
193	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
194	Taming the Reactivity of Monoterpene Synthases To Guide Regioselective Product Hydroxylation. ChemBioChem, 2020, 21, 985-990.	1.3	13
195	COVID19 - Computational Chemists Meet the Moment. Journal of Chemical Information and Modeling, 2020, 60, 5724-5726.	2.5	13
196	Active-site dynamics of ASADH?A bacterial biosynthetic enzyme. International Journal of Quantum Chemistry, 1999, 73, 137-146.	1.0	12
197	Benchmarking quantum mechanical methods for calculating reaction energies of reactions catalyzed by enzymes. PeerJ Physical Chemistry, 0, 2, e8.	0.0	12
198	Identification of Potent DNA Gyrase Inhibitors Active against Mycobacterium tuberculosis. Journal of Chemical Information and Modeling, 2022, 62, 1680-1690.	2.5	12

#	Article	IF	Citations
199	Computational Enzymology. Methods in Molecular Biology, 2013, 924, 67-89.	0.4	11
200	Nonempirical Energetic Analysis of Reactivity and Covalent Inhibition of Fatty Acid Amide Hydrolase. Journal of Physical Chemistry B, 2013, 117, 6656-6666.	1.2	11
201	Quantum Mechanics/Molecular Mechanics Simulations Identify the Ring-Opening Mechanism of Creatininase. Biochemistry, 2017, 56, 6377-6388.	1.2	11
202	Catalytic mechanism of the colistin resistance protein MCR-1. Organic and Biomolecular Chemistry, 2021, 19, 3813-3819.	1.5	11
203	The emerging potential of interactive virtual reality in drug discovery. Expert Opinion on Drug Discovery, 2022, 17, 685-698.	2.5	11
204	In pursuit of an accurate spatial and temporal model of biomolecules at the atomistic level: a perspective on computer simulation. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 162-172.	2.5	10
205	Combined Quantum Mechanics and Molecular Mechanics Studies of Enzymatic Reaction Mechanisms. Advances in Protein Chemistry and Structural Biology, 2018, 113, 1-32.	1.0	10
206	In silico study directed towards identification of the key structural features of GyrB inhibitors targeting MTB DNA gyrase: HQSAR, CoMSIA and molecular dynamics simulations. SAR and QSAR in Environmental Research, 2019, 30, 775-800.	1.0	10
207	Resistance to the â€œlast resortâ€•antibiotic colistin: a single-zinc mechanism for phosphointermediate formation in MCR enzymes. Chemical Communications, 2020, 56, 6874-6877.	2.2	10
208	Multiscale Workflow for Modeling Ligand Complexes of Zinc Metalloproteins. Journal of Chemical Information and Modeling, 2021, 61, 5658-5672.	2.5	10
209	Introduction. Biomolecular simulation. Journal of the Royal Society Interface, 2008, 5, 169-172.	1.5	9
210	Applications and Advances of QM/MM Methods in Computational Enzymology. Annual Reports in Computational Chemistry, 2008, , 155-169.	0.9	9
211	QM/MM simulations indicate that Asp185 is the likely catalytic base in the enzymatic reaction of HIV-1 reverse transcriptase. MedChemComm, 2014, 5, 593.	3.5	9
212	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
213	Multiscale Simulations Identify Origins of Differential Carbapenem Hydrolysis by the OXA-48 Î²-Lactamase. ACS Catalysis, 2022, 12, 4534-4544.	5.5	9
214	Generalized Born Implicit Solvent Models Do Not Reproduce Secondary Structures of De Novo Designed Glu/Lys Peptides. Journal of Chemical Theory and Computation, 2022, 18, 4070-4076.	2.3	9
215	MECHANISTIC STUDY OF HIV-1 REVERSE TRANSCRIPTASE AT THE ACTIVE SITE BASED ON QM/MM METHOD. Journal of Theoretical and Computational Chemistry, 2004, 03, 491-500.	1.8	8
216	The reaction mechanism of Zika virus NS2B/NS3 serine protease inhibition by dipeptidyl aldehyde: a QM/MM study. Physical Chemistry Chemical Physics, 2019, 21, 14945-14956.	1.3	8

#	Article	IF	Citations
217	Electronic structure benchmark calculations of <scp>CO₂</scp> fixing elementary chemical steps in <scp>RuBisCO</scp> using the projectorâ€based embedding approach. Journal of Computational Chemistry, 2020, 41, 2151-2157.	1.5	8
218	Substrate promiscuity of a de novo designed peroxidase. Journal of Inorganic Biochemistry, 2021, 217, 111370.	1.5	8
219	A multiscale approach to predict the binding mode of metallo betaâ€lactamase inhibitors. Proteins: Structure, Function and Bioinformatics, 2022, 90, 372-384.	1.5	8
220	QM/MM Molecular Modeling Reveals Mechanism Insights into Flavin Peroxide Formation in Bacterial Luciferase. Journal of Chemical Information and Modeling, 2022, 62, 399-411.	2.5	8
221	Quantum-Mechanical/Molecular-Mechanical Methods in Medicinal Chemistry. Methods and Principles in Medicinal Chemistry, 2005, , 177-198.	0.3	7
222	Dispelling the effects of a sorceress in enzyme catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 2328-2330.	3.3	7
223	Frontispiz: Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARSâ€CoVâ€2 Spike Protein. Angewandte Chemie, 2021, 133, .	1.6	7
224	Exploring human-guided strategies for reaction network exploration: Interactive molecular dynamics in virtual reality as a tool for citizen scientists. Journal of Chemical Physics, 2021, 155, 154106.	1.2	7
225	Comment on â€œMolecular dynamics DFT:B3LYP study of guanosinetriphosphate conversion into guanosinemonophosphate upon Mg2+chelation of Î± and Î² phosphate oxygens of the triphosphate tailâ€•by Alexander A. Tulub, Phys. Chem. Chem. Phys., 2006, 8, 2187. Physical Chemistry Chemical Physics, 2006, 8, 5366-5367.	1.3	6
226	Comment on â€œA stationary-wave model of enzyme catalysisâ€•by Carlo Canepa. Journal of Computational Chemistry, 2011, 32, 368-369.	1.5	6
227	Quantum Mechanics/Molecular Mechanics Simulations Show Saccharide Distortion is Required for Reaction in Hen Eggâ€White Lysozyme. Chemistry - A European Journal, 2019, 25, 764-768.	1.7	6
228	Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARSâ€CoVâ€2 Spike Protein**. Angewandte Chemie, 2021, 133, 7174-7186.	1.6	6
229	A conserved arginine with nonâ€conserved function is a key determinant of agonist selectivity in Î±7 nicotinic ACh receptors. British Journal of Pharmacology, 2021, 178, 1651-1668.	2.7	6
230	Exploration of the structural requirements of Aurora Kinase B inhibitors by a combined QSAR, modelling and molecular simulation approach. Scientific Reports, 2021, 11, 18707.	1.6	6
231	Crystallography and QM/MM Simulations Identify Preferential Binding of Hydrolyzed Carbapenem and Penem Antibiotics to the L1 Metallo-Î²-Lactamase in the Imine Form. Journal of Chemical Information and Modeling, 2021, , .	2.5	5
232	Science to enable the circular economy. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20200060.	1.6	4
233	Chapter 11. QM/MM Methods for Simulating Enzyme Reactions. RSC Theoretical and Computational Chemistry Series, 2016, , 375-403.	0.7	4
234	Modeling the Citrate Synthase Reaction: QM/MM and Small Model Calculations. ACS Symposium Series, 1999, , 448-461.	0.5	3

#	Article	IF	Citations
235	Optimal control design of laser pulses for mode specific vibrational excitation in an enzymeâ€“substrate complex. Chemical Physics Letters, 2010, 491, 230-236.	1.2	3
236	Insights into conformational changes of procarboxypeptidase A and B from simulations: a plausible explanation for different intrinsic activity. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	3
237	Simulations of Shikimate Dehydrogenase from Mycobacterium tuberculosis in Complex with 3-Dehydroshikimate and NADPH Suggest Strategies for MtbSDH Inhibition. Journal of Chemical Information and Modeling, 2019, 59, 1422-1433.	2.5	3
238	Acetylâ€CoA enolization in citrate synthase: A quantum mechanical/molecular mechanical (QM/MM) study. Proteins: Structure, Function and Bioinformatics, 1997, 27, 9-25.	1.5	3
239	Chapter 11. QM/MM Studies of Cytochrome P450 Systems: Application to Drug Metabolism. , 0, , 366-399.		2
240	Molecular Dynamics, Quantum Mechanics, and Combined Quantum Mechanics/Molecular Mechanics Methods for Drug Discovery and Development. , 2017, , 51-66.		1
241	Discovery of novel and potent InhA inhibitors by an in silico screening and pharmacokinetic prediction. Future Medicinal Chemistry, 2022, 14, 717-729.	1.1	1
242	Computational Enzymology: Insights into Enzyme Mechanism and Catalysis from Modelling. Challenges and Advances in Computational Chemistry and Physics, 2007, , 275-304.	0.6	0
243	QM/MM Study on Cleavage Mechanism Catalyzed by Zika Virus NS2B/NS3 Serine Protease. Biophysical Journal, 2019, 116, 559a.	0.2	0
244	Frontispiece: Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARSâ€CoVâ€2 Spike Protein. Angewandte Chemie - International Edition, 2021, 60, .	7.2	0
245	Enzyme Dynamics and Catalysis: Insights from Simulations. Challenges and Advances in Computational Chemistry and Physics, 2010, , 375-395.	0.6	0