Adrian J Mulholland

List of Publications by Year in Descending Order

249 papers	9,158 citations	54 h-index	82 g-index
314 ext. papers	10,720 ext. citations	7 avg, IF	6.59 L-index

#	Paper	IF	Citations
249	QM/MM Molecular Modeling Reveals Mechanism Insights into Flavin Peroxide Formation in Bacterial Luciferase.. *Journal of Chemical Information and Modeling*, **2022**,	6.1	2
248	Structural insights in cell-type specific evolution of intra-host diversity by SARS-CoV-2.. *Nature Communications*, **2022**, 13, 222	17.4	2
247	Mechanistic Insights into the Ligand-Induced Unfolding of an RNA G-Quadruplex.. *Journal of the American Chemical Society*, **2022**,	16.4	2
246	Multiscale Simulations Identify Origins of Differential Carbapenem Hydrolysis by the OXA-48 -Lactamase.. *ACS Catalysis*, **2022**, 12, 4534-4544	13.1	0
245	Impact of Warhead Modulations on the Covalent Inhibition of SARS-CoV-2 M Explored by QM/MM Simulations.. *ACS Catalysis*, **2022**, 12, 698-708	13.1	2
244	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*, **2021**,	6.8	2
243	Multiscale Workflow for Modeling Ligand Complexes of Zinc Metalloproteins. *Journal of Chemical Information and Modeling*, **2021**, 61, 5658-5672	6.1	1
242	#COVIDisAirborne: AI-Enabled Multiscale Computational Microscopy of Delta SARS-CoV-2 in a Respiratory Aerosol **2021**,		9
241	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	3.9	2
240	Frontispiz: Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARS-CoV-2 Spike Protein. *Angewandte Chemie*, **2021**, 133,	3.6	3
239	Allosteric communication in class A -lactamases occurs via cooperative coupling of loop dynamics. *ELife*, **2021**, 10,	8.9	18
238	Structural resolution of switchable states of a de novo peptide assembly. *Nature Communications*, **2021**, 12, 1530	17.4	8
237	A potential interaction between the SARS-CoV-2 spike protein and nicotinic acetylcholine receptors. *Biophysical Journal*, **2021**, 120, 983-993	2.9	18
236	Designing better enzymes: Insights from directed evolution. *Current Opinion in Structural Biology*, **2021**, 67, 212-218	8.1	14
235	Substrate promiscuity of a de novo designed peroxidase. *Journal of Inorganic Biochemistry*, **2021**, 217, 111370	4.2	2
234	Constructing ion channels from water-soluble -helical barrels. *Nature Chemistry*, **2021**, 13, 643-650	17.6	14
233	Dissecting the low catalytic capability of flavin-dependent halogenases. *Journal of Biological Chemistry*, **2021**, 296, 100068	5.4	6

232	Catalytic mechanism of the colistin resistance protein MCR-1. *Organic and Biomolecular Chemistry*, **2021**, 19, 3813-3819	3.9	6
231	Natural variants modify Klebsiella pneumoniae carbapenemase (KPC) acyl-enzyme conformational dynamics to extend antibiotic resistance. *Journal of Biological Chemistry*, **2021**, 296, 100126	5.4	8
230	Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARS-CoV-2 Spike Protein*. *Angewandte Chemie - International Edition*, **2021**, 60, 7098-7110	16.4	37
229	Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARS-CoV-2 Spike Protein**. *Angewandte Chemie*, **2021**, 133, 7174-7186	3.6	4
228	A conserved arginine with non-conserved function is a key determinant of agonist selectivity in α7 nicotinic ACh receptors. *British Journal of Pharmacology*, **2021**, 178, 1651-1668	8.6	1
227	A robust and stereocomplementary panel of ene-reductase variants for gram-scale asymmetric hydrogenation. *Molecular Catalysis*, **2021**, 502, 111404	3.3	5
226	Dynamical nonequilibrium molecular dynamics reveals the structural basis for allostery and signal propagation in biomolecular systems. *European Physical Journal B*, **2021**, 94, 144	1.2	5
225	Evolution of dynamical networks enhances catalysis in a designer enzyme. *Nature Chemistry*, **2021**, 13, 1017-1022	17.6	8
224	Rigidifying a Enzyme Increases Activity and Induces a Negative Activation Heat Capacity. *ACS Catalysis*, **2021**, 11, 11532-11541	13.1	4
223	Exploration of the structural requirements of Aurora Kinase B inhibitors by a combined QSAR, modelling and molecular simulation approach. *Scientific Reports*, **2021**, 11, 18707	4.9	3
222	A multiscale approach to predict the binding mode of metallo beta-lactamase inhibitors. *Proteins: Structure, Function and Bioinformatics*, **2021**,	4.2	3
221	Molecular dynamics simulations support the hypothesis that the brGDGT paleothermometer is based on homeoviscous adaptation. *Geochimica Et Cosmochimica Acta*, **2021**, 312, 44-56	5.5	6
220	Discovery of SARS-CoV-2 M peptide inhibitors from modelling substrate and ligand binding. *Chemical Science*, **2021**, 12, 13686-13703	9.4	14
219	Mechanism of covalent binding of ibrutinib to Bruton's tyrosine kinase revealed by QM/MM calculations. *Chemical Science*, **2021**, 12, 5511-5516	9.4	10
218	Resistance to the "last resort" antibiotic colistin: a single-zinc mechanism for phosphointermediate formation in MCR enzymes. *Chemical Communications*, **2020**, 56, 6874-6877	5.8	5
217	Small Changes in Hydration Determine Cephalosporinase Activity of OXA-48 β-Lactamases. *ACS Catalysis*, **2020**, 10, 6188-6196	13.1	6
216	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	11.5	16
215	Interactive molecular dynamics in virtual reality for accurate flexible protein-ligand docking. *PLoS ONE*, **2020**, 15, e0228461	3.7	17

214	Electronic structure benchmark calculations of CO fixing elementary chemical steps in RuBisCO using the projector-based embedding approach. *Journal of Computational Chemistry*, **2020**, 41, 2151-2157	3.5	5
213	Enzyme evolution and the temperature dependence of enzyme catalysis. *Current Opinion in Structural Biology*, **2020**, 65, 96-101	8.1	18
212	Temperature, Dynamics, and Enzyme-Catalyzed Reaction Rates. *Annual Review of Biophysics*, **2020**, 49, 163-180	21.1	19
211	Multiscale simulation approaches to modeling drug-protein binding. *Current Opinion in Structural Biology*, **2020**, 61, 213-221	8.1	17
210	Cyclic boronates as versatile scaffolds for KPC-2 β-lactamase inhibition. *RSC Medicinal Chemistry*, **2020**, 11, 491-496	3.5	14
209	A Community Letter Regarding Sharing Biomolecular Simulation Data for COVID-19. *Journal of Chemical Information and Modeling*, **2020**, 60, 2653-2656	6.1	45
208	Visible-light photoswitching of ligand binding mode suggests G-quadruplex DNA as a target for photopharmacology. *Chemical Communications*, **2020**, 56, 5186-5189	5.8	15
207	Simulations support the interaction of the SARS-CoV-2 spike protein with nicotinic acetylcholine receptors **2020**,		10
206	Taming the Reactivity of Monoterpene Synthases To Guide Regioselective Product Hydroxylation. *ChemBioChem*, **2020**, 21, 985-990	3.8	8
205	IMPRESSION - prediction of NMR parameters for 3-dimensional chemical structures using machine learning with near quantum chemical accuracy. *Chemical Science*, **2020**, 11, 508-515	9.4	34
204	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	6.1	11
203	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	6.1	16
202	Science to enable the circular economy. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2020**, 378, 20200060	3	3
201	Biomolecular Simulations in the Time of COVID19, and After. *Computing in Science and Engineering*, **2020**, 22, 30-36	1.5	16
200	Free fatty acid binding pocket in the locked structure of SARS-CoV-2 spike protein. *Science*, **2020**, 370, 725-730	33.3	182
199	Mechanism of inhibition of SARS-CoV-2 M by peptidyl Michael acceptor explained by QM/MM simulations and design of new derivatives with tunable chemical reactivity. *Chemical Science*, **2020**, 12, 1433-1444	9.4	50
198	Enhanced sampling molecular dynamics simulations correctly predict the diverse activities of a series of stiff-stilbene G-quadruplex DNA ligands. *Chemical Science*, **2020**, 12, 1415-1426	9.4	6
197	Molecular Dynamics Simulation Framework to Probe the Binding Hypothesis of CYP3A4 Inhibitors. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	6

196	Limitations of Ligand-Only Approaches for Predicting the Reactivity of Covalent Inhibitors. *Journal of Chemical Information and Modeling*, **2019**, 59, 4220-4227	6.1	10
195	A Photoresponsive Stiff-Stilbene Ligand Fuels the Reversible Unfolding of G-Quadruplex DNA. *Angewandte Chemie - International Edition*, **2019**, 58, 4334-4338	16.4	32
194	A Photoresponsive Stiff-Stilbene Ligand Fuels the Reversible Unfolding of G-Quadruplex DNA. *Angewandte Chemie*, **2019**, 131, 4378-4382	3.6	13
193	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	3.6	6
192	Identification of the Initial Steps in Signal Transduction in the 42 Nicotinic Receptor: Insights from Equilibrium and Nonequilibrium Simulations. *Structure*, **2019**, 27, 1171-1183.e3	5.2	9
191	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	3.9	40
190	Visualizing protein-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	4.2	9
189	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	3.4	13
188	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	6.1	1
187	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	6.1	17
186	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1393	7.9	69
185	Experiment and Simulation Reveal How Mutations in Functional Plasticity Regions Guide Plant Monoterpene Synthase Product Outcome. *ACS Catalysis*, **2019**, 8, 3780-3791	13.1	20
184	Molecular Basis of Class A Lactamase Inhibition by Relebactam. *Antimicrobial Agents and Chemotherapy*, **2019**, 63,	5.9	26
183	Emergence of a Negative Activation Heat Capacity during Evolution of a Designed Enzyme. *Journal of the American Chemical Society*, **2019**, 141, 11745-11748	16.4	20
182	Teaching Enzyme Catalysis Using Interactive Molecular Dynamics in Virtual Reality. *Journal of Chemical Education*, **2019**, 96, 2488-2496	2.4	56
181	An Efficient Computational Assay for Lactam Antibiotic Breakdown by Class A Lactamases. *Journal of Chemical Information and Modeling*, **2019**, 59, 3365-3369	6.1	12
180	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	3.5	7
179	BioSimSpace: An interoperable Python framework for biomolecular simulation. *Journal of Open Source Software*, **2019**, 4, 1831	5.2	12

178	A General Mechanism for Signal Propagation in the Nicotinic Acetylcholine Receptor Family. *Journal of the American Chemical Society*, **2019**, 141, 19953-19958	16.4	13
177	Quantum Mechanics/Molecular Mechanics Simulations Show Saccharide Distortion is Required for Reaction in Hen Egg-White Lysozyme. *Chemistry - A European Journal*, **2019**, 25, 764-768	4.8	5
176	P450-Catalyzed Regio- and Diastereoselective Steroid Hydroxylation: Efficient Directed Evolution Enabled by Mutability Landscaping. *ACS Catalysis*, **2018**, 8, 3395-3410	13.1	81
175	Multiscale analysis of enantioselectivity in enzyme-catalysed 'lethal synthesis' using projector-based embedding. *Royal Society Open Science*, **2018**, 5, 171390	3.3	17
174	Multiscale Methods in Drug Design Bridge Chemical and Biological Complexity in the Search for Cures. *Nature Reviews Chemistry*, **2018**, 2,	34.6	72
173	Dynamical origins of heat capacity changes in enzyme-catalysed reactions. *Nature Communications*, **2018**, 9, 1177	17.4	41
172	Structural Insights from Molecular Dynamics Simulations of Tryptophan 7-Halogenase and Tryptophan 5-Halogenase. *ACS Omega*, **2018**, 3, 4847-4859	3.9	13
171	Biocatalytic Routes to Lactone Monomers for Polymer Production. *Biochemistry*, **2018**, 57, 1997-2008	3.2	28
170	Combined Quantum Mechanics and Molecular Mechanics Studies of Enzymatic Reaction Mechanisms. *Advances in Protein Chemistry and Structural Biology*, **2018**, 113, 1-32	5.3	5
169	Unlocking Nicotinic Selectivity via Direct C-H Functionalization of (−)-Cytisine. *CheM*, **2018**, 4, 1710-1725	16.2	20
168	Maintaining and breaking symmetry in homomeric coiled-coil assemblies. *Nature Communications*, **2018**, 9, 4132	17.4	25
167	Loop Motion in Triosephosphate Isomerase Is Not a Simple Open and Shut Case. *Journal of the American Chemical Society*, **2018**, 140, 15889-15903	16.4	36
166	A Multiscale Simulation Approach to Modeling Drug-Protein Binding Kinetics. *Journal of Chemical Theory and Computation*, **2018**, 14, 6093-6101	6.4	21
165	Multiscale Simulations of Clavulanate Inhibition Identify the Reactive Complex in Class A β-Lactamases and Predict the Efficiency of Inhibition. *Biochemistry*, **2018**, 57, 3560-3563	3.2	14
164	QM/MM simulations identify the determinants of catalytic activity differences between type II dehydroquinase enzymes. *Organic and Biomolecular Chemistry*, **2018**, 16, 4443-4455	3.9	14
163	Understanding Complex Mechanisms of Enzyme Reactivity: The Case of Limonene-1,2-Epoxide Hydrolases. *ACS Catalysis*, **2018**, 8, 5698-5707	13.1	17
162	Sampling molecular conformations and dynamics in a multiuser virtual reality framework. *Science Advances*, **2018**, 4, eaat2731	14.3	64
161	De Novo-Designed α-Helical Barrels as Receptors for Small Molecules. *ACS Synthetic Biology*, **2018**, 7, 1808-1816	5.7	33

160	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	4.9	78
159	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	6.4	9
158	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	4.2	10
157	Molecular Dynamics, Quantum Mechanics, and Combined Quantum Mechanics/Molecular Mechanics Methods for Drug Discovery and Development **2017**, 51-66		1
156	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	3.4	12
155	Construction and in vivo assembly of a catalytically proficient and hyperthermostable de novo enzyme. *Nature Communications*, **2017**, 8, 358	17.4	66
154	Structural Basis of Catalysis in the Bacterial Monoterpene Synthases Linalool Synthase and 1,8-Cineole Synthase. *ACS Catalysis*, **2017**, 7, 6268-6282	13.1	31
153	Mechanistic Insights into the Reaction of Chlorination of Tryptophan Catalyzed by Tryptophan 7-Halogenase. *Scientific Reports*, **2017**, 7, 17395	4.9	19
152	Quantum Mechanics/Molecular Mechanics Simulations Identify the Ring-Opening Mechanism of Creatininase. *Biochemistry*, **2017**, 56, 6377-6388	3.2	10
151	Elucidation of Nonadditive Effects in Protein-Ligand Binding Energies: Thrombin as a Case Study. *Journal of Physical Chemistry B*, **2016**, 120, 5340-50	3.4	22
150	Dispelling the effects of a sorceress in enzyme catalysis. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 2328-30	11.5	4
149	On the Temperature Dependence of Enzyme-Catalyzed Rates. *Biochemistry*, **2016**, 55, 1681-8	3.2	138
148	Chapter 11:QM/MM Methods for Simulating Enzyme Reactions. *RSC Theoretical and Computational Chemistry Series*, **2016**, 375-403	1.2	4
147	Quantum Mechanics/Molecular Mechanics Modeling of Drug Metabolism: Mexiletine N-Hydroxylation by Cytochrome P450 1A2. *Chemical Research in Toxicology*, **2016**, 29, 963-71	4	25
146	The Catalytic Mechanism of a Natural Diels-Alderase Revealed in Molecular Detail. *Journal of the American Chemical Society*, **2016**, 138, 6095-8	16.4	112
145	A Projector-Embedding Approach for Multiscale Coupled-Cluster Calculations Applied to Citrate Synthase. *Journal of Chemical Theory and Computation*, **2016**, 12, 2689-97	6.4	51
144	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, 162-72		9
143	Combined quantum mechanics/molecular mechanics (QM/MM) simulations for protein-ligand complexes: free energies of binding of water molecules in influenza neuraminidase. *Journal of Physical Chemistry B*, **2015**, 119, 997-1001	3.4	22

142	Structure and Function in Homodimeric Enzymes: Simulations of Cooperative and Independent Functional Motions. *PLoS ONE*, **2015**, 10, e0133372	3.7	20
141	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, 713-22	6.4	19
140	Reaction mechanism of N-acetylneuraminic acid lyase revealed by a combination of crystallography, QM/MM simulation, and mutagenesis. *ACS Chemical Biology*, **2014**, 9, 1025-32	4.9	36
139	Large-Scale Density Functional Theory Transition State Searching in Enzymes. *Journal of Physical Chemistry Letters*, **2014**, 5, 3614-9	6.4	43
138	QM/MM simulations as an assay for carbapenemase activity in class A β-lactamases. *Chemical Communications*, **2014**, 50, 14736-9	5.8	30
137	A catalytic role for methionine revealed by a combination of computation and experiments on phosphite dehydrogenase. *Chemical Science*, **2014**, 5, 2191-2199	9.4	28
136	Rapid decomposition and visualisation of protein-ligand binding free energies by residue and by water. *Faraday Discussions*, **2014**, 169, 477-99	3.6	42
135	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, 1608-22	6.4	48
134	QM/MM simulations indicate that Asp185 is the likely catalytic base in the enzymatic reaction of HIV-1 reverse transcriptase. *MedChemComm*, **2014**, 5, 593	5	6
133	Role of active site residues in promoting cobalt-carbon bond homolysis in adenosylcobalamin-dependent mutases revealed through experiment and computation. *Biochemistry*, **2014**, 53, 169-77	3.2	16
132	Trends in predicted chemoselectivity of cytochrome P450 oxidation: B3LYP barrier heights for epoxidation and hydroxylation reactions. *Journal of Molecular Graphics and Modelling*, **2014**, 52, 30-5	2.8	22
131	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, 4771-83	3.4	32
130	Comparison of DFT and ab initio QM/MM methods for modelling reaction in chorismate synthase. *Chemical Physics Letters*, **2014**, 608, 380-385	2.5	19
129	A multiscale approach to modelling drug metabolism by membrane-bound cytochrome P450 enzymes. *PLoS Computational Biology*, **2014**, 10, e1003714	5	38
128	QM/MM modelling of drug-metabolizing enzymes. *Current Topics in Medicinal Chemistry*, **2014**, 14, 1339-47	3	18
127	Conformational change and ligand binding in the aristolochene synthase catalytic cycle. *Biochemistry*, **2013**, 52, 8094-105	3.2	29
126	Analysis and assay of oseltamivir-resistant mutants of influenza neuraminidase via direct observation of drug unbinding and rebinding in simulation. *Biochemistry*, **2013**, 52, 8150-64	3.2	20
125	Computational enzymology. *Methods in Molecular Biology*, **2013**, 924, 67-89	1.4	11

124	Conformational effects on the pro-S hydrogen abstraction reaction in cyclooxygenase-1: an integrated QM/MM and MD study. *Biophysical Journal*, **2013**, 104, L5-7	2.9	21
123	Quantum mechanics/molecular mechanics modeling of fatty acid amide hydrolase reactivation distinguishes substrate from irreversible covalent inhibitors. *Journal of Medicinal Chemistry*, **2013**, 56, 2500-12	8.3	28
122	Combined quantum mechanics/molecular mechanics (QM/MM) methods in computational enzymology. *Biochemistry*, **2013**, 52, 2708-28	3.2	388
121	Quantum mechanics/molecular mechanics modeling of regioselectivity of drug metabolism in cytochrome P450 2C9. *Journal of the American Chemical Society*, **2013**, 135, 8001-15	16.4	96
120	Nonempirical energetic analysis of reactivity and covalent inhibition of fatty acid amide hydrolase. *Journal of Physical Chemistry B*, **2013**, 117, 6656-66	3.4	10
119	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, 16344-9	11.5	105
118	QM/MM modelling of ketosteroid isomerase reactivity indicates that active site closure is integral to catalysis. *FEBS Journal*, **2013**, 280, 3120-31	5.7	28
117	Computational assay of H7N9 influenza neuraminidase reveals R292K mutation reduces drug binding affinity. *Scientific Reports*, **2013**, 3, 3561	4.9	34
116	The basis for carbapenem hydrolysis by class A β-lactamases: a combined investigation using crystallography and simulations. *Journal of the American Chemical Society*, **2012**, 134, 18275-85	16.4	60
115	Mechanism of C-terminal intein cleavage in protein splicing from QM/MM molecular dynamics simulations. *Organic and Biomolecular Chemistry*, **2012**, 10, 1207-18	3.9	24
114	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, 4637-45	6.4	70
113	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, 4364-75	3.2	33
112	Protein dynamics and enzyme catalysis: the ghost in the machine?. *Biochemical Society Transactions*, **2012**, 40, 515-21	5.1	16
111	A practical guide to modelling enzyme-catalysed reactions. *Chemical Society Reviews*, **2012**, 41, 3025-38	58.5	124
110	Enzyme dynamics and catalysis in the mechanism of DNA polymerase. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	14
109	Insights into conformational changes of procarboxypeptidase A and B from simulations: a plausible explanation for different intrinsic activity. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	2
108	Determinants of reactivity and selectivity in soluble epoxide hydrolase from quantum mechanics/molecular mechanics modeling. *Biochemistry*, **2012**, 51, 1774-86	3.2	54
107	Taking Ockham's razor to enzyme dynamics and catalysis. *Nature Chemistry*, **2012**, 4, 169-76	17.6	186

106	Does compound I vary significantly between isoforms of cytochrome P450?. *Journal of the American Chemical Society*, **2011**, 133, 15464-74	16.4	165
105	A water-swap reaction coordinate for the calculation of absolute protein-ligand binding free energies. *Journal of Chemical Physics*, **2011**, 134, 054114	3.9	53
104	Analysis of chorismate mutase catalysis by QM/MM modelling of enzyme-catalysed and uncatalysed reactions. *Organic and Biomolecular Chemistry*, **2011**, 9, 1578-90	3.9	54
103	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, 2375-83	2	17
102	Comment on "A stationary-wave model of enzyme catalysis" by Carlo Canepa. *Journal of Computational Chemistry*, **2011**, 32, 368-9; author reply 370-1	3.5	6
101	Lethal Synthesis of Fluorocitrate by Citrate Synthase Explained through QM/MM Modeling. *Angewandte Chemie*, **2011**, 123, 10533-10535	3.6	3
100	"Lethal synthesis" of fluorocitrate by citrate synthase explained through QM/MM modeling. *Angewandte Chemie - International Edition*, **2011**, 50, 10349-51	16.4	17
99	Understanding the role of carbamate reactivity in fatty acid amide hydrolase inhibition by QM/MM mechanistic modelling. *Chemical Communications*, **2011**, 47, 2517-9	5.8	21
98	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, 4697-711	3.2	49
97	Protein dynamics and enzyme catalysis: insights from simulations. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2011**, 1814, 1077-92	4	62
96	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, 6050-5	11.5	82
95	QM and QM/MM Approaches to Evaluating Binding Affinities **2010**, 725-752		1
94	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, 2948-60	6.4	53
93	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	6.4	47
92	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	6.4	137
91	Computational enzymology. *Chemical Communications*, **2010**, 46, 2354-72	5.8	90
90	Compound I reactivity defines alkene oxidation selectivity in cytochrome P450cam. *Journal of Physical Chemistry B*, **2010**, 114, 1156-62	3.4	98
89	Investigations of enzyme-catalysed reactions with combined quantum mechanics/molecular mechanics (QM/MM) methods. *International Reviews in Physical Chemistry*, **2010**, 29, 65-133	7	89

88	Testing high-level QM/MM methods for modeling enzyme reactions: acetyl-CoA deprotonation in citrate synthase. *Journal of Physical Chemistry B*, **2010**, 114, 11303-14	3.4	54
87	Optimal control design of laser pulses for mode specific vibrational excitation in an enzyme–substrate complex. *Chemical Physics Letters*, **2010**, 491, 230-236	2.5	3
86	Computer simulations of quantum tunnelling in enzyme-catalysed hydrogen transfer reactions. *Interdisciplinary Sciences, Computational Life Sciences*, **2010**, 2, 78-97	3.5	15
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