Adrian J Mulholland

List of Publications by Citations

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	Combined quantum mechanics/molecular mechanics (QM/MM) methods in computational enzymology. *Biochemistry*, **2013**, 52, 2708-28	3.2	388
248	Atomic description of an enzyme reaction dominated by proton tunneling. *Science*, **2006**, 312, 237-41	33.3	278
247	High-accuracy computation of reaction barriers in enzymes. *Angewandte Chemie - International Edition*, **2006**, 45, 6856-9	16.4	223
246	Taking Ockham's razor to enzyme dynamics and catalysis. *Nature Chemistry*, **2012**, 4, 169-76	17.6	186
245	Free fatty acid binding pocket in the locked structure of SARS-CoV-2 spike protein. *Science*, **2020**, 370, 725-730	33.3	182
244	Does compound I vary significantly between isoforms of cytochrome P450?. *Journal of the American Chemical Society*, **2011**, 133, 15464-74	16.4	165
243	Modelling enzyme reaction mechanisms, specificity and catalysis. *Drug Discovery Today*, **2005**, 10, 1393-1402	8.8	155
242	Electronic structure of compound I in human isoforms of cytochrome P450 from QM/MM modeling. *Journal of the American Chemical Society*, **2005**, 127, 12900-8	16.4	147
241	On the Temperature Dependence of Enzyme-Catalyzed Rates. *Biochemistry*, **2016**, 55, 1681-8	3.2	138
240	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
239	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	16.4	132
238	A practical guide to modelling enzyme-catalysed reactions. *Chemical Society Reviews*, **2012**, 41, 3025-38	58.5	124
237	Aromatic hydroxylation by cytochrome P450: model calculations of mechanism and substituent effects. *Journal of the American Chemical Society*, **2003**, 125, 15004-5	16.4	119
236	Mechanisms of antibiotic resistance: QM/MM modeling of the acylation reaction of a class A beta-lactamase with benzylpenicillin. *Journal of the American Chemical Society*, **2005**, 127, 4454-65	16.4	116
235	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
234	Mechanism and structure-reactivity relationships for aromatic hydroxylation by cytochrome P450. *Organic and Biomolecular Chemistry*, **2004**, 2, 2998-3005	3.9	107
233	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	16.4	106

232	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
231	Compound I reactivity defines alkene oxidation selectivity in cytochrome P450cam. *Journal of Physical Chemistry B*, **2010**, 114, 1156-62	3.4	98
230	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
229	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, 968-80	3.9	94
228	Computational enzymology. *Chemical Communications*, **2010**, 46, 2354-72	5.8	90
227	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
226	Acetyl-CoA enolization in citrate synthase: A quantum mechanical/molecular mechanical (QM/MM) study. *Proteins: Structure, Function and Bioinformatics*, **1997**, 27, 9-25	4.2	89
225	Differential transition-state stabilization in enzyme catalysis: 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, 16148-59	16.4	88
224	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
223	An efficient method for the calculation of quantum mechanics/molecular mechanics free energies. *Journal of Chemical Physics*, **2008**, 128, 014109	3.9	82
222	P450-Catalyzed Regio- and Diastereoselective Steroid Hydroxylation: Efficient Directed Evolution Enabled by Mutability Landscaping. *ACS Catalysis*, **2018**, 8, 3395-3410	13.1	81
221	QM/MM modeling of benzene hydroxylation in human cytochrome P450 2C9. *Journal of Physical Chemistry A*, **2008**, 112, 13149-56	2.8	79
220	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
219	Quantum mechanical/molecular mechanical free energy simulations of the glutathione S-transferase (M1-1) reaction with phenanthrene 9,10-oxide. *Journal of the American Chemical Society*, **2002**, 124, 9926-36	16.4	76
218	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	16.4	76
217	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**, 5068-70	5.8	74
216	Multiscale Methods in Drug Design Bridge Chemical and Biological Complexity in the Search for Cures. *Nature Reviews Chemistry*, **2018**, 2,	34.6	72
215	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

214	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1393	7.9	69
213	Conformational effects in enzyme catalysis: reaction via a high energy conformation in fatty acid amide hydrolase. *Biophysical Journal*, **2007**, 92, L20-2	2.9	69
212	Ab Initio QM/MM Modeling of the Hydroxylation Step in p-Hydroxybenzoate Hydroxylase. *Journal of Physical Chemistry B*, **2003**, 107, 2118-2126	3.4	67
211	Construction and in vivo assembly of a catalytically proficient and hyperthermostable de novo enzyme. *Nature Communications*, **2017**, 8, 358	17.4	66
210	Insights into enzyme catalysis from QM/MM modelling: transition state stabilization in chorismate mutase. *Molecular Physics*, **2003**, 101, 2695-2714	1.7	66
209	Sampling molecular conformations and dynamics in a multiuser virtual reality framework. *Science Advances*, **2018**, 4, eaat2731	14.3	64
208	Identification of Glu166 as the general base in the acylation reaction of class A beta-lactamases through QM/MM modeling. *Journal of the American Chemical Society*, **2003**, 125, 9590-1	16.4	63
207	Protein dynamics and enzyme catalysis: insights from simulations. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2011**, 1814, 1077-92	4	62
206	QM/MM simulations predict a covalent intermediate in the hen egg white lysozyme reaction with its natural substrate. *Chemical Communications*, **2008**, 4425-7	5.8	62
205	Biomolecular simulation and modelling: status, progress and prospects. *Journal of the Royal Society Interface*, **2008**, 5 Suppl 3, S173-90	4.1	62
204	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
203	QM/MM modelling of oleamide hydrolysis in fatty acid amide hydrolase (FAAH) reveals a new mechanism of nucleophile activation. *Chemical Communications*, **2005**, 4399-401	5.8	59
202	Hydrogen tunnelling in enzyme-catalysed H-transfer reactions: flavoprotein and quinoprotein systems. *Philosophical Transactions of the Royal Society B: Biological Sciences*, **2006**, 361, 1375-86	5.8	59
201	Molecular mechanisms of antibiotic resistance: QM/MM modelling of deacylation in a class A beta-lactamase. *Organic and Biomolecular Chemistry*, **2006**, 4, 206-10	3.9	59
200	Identification of productive inhibitor binding orientation in fatty acid amide hydrolase (FAAH) by QM/MM mechanistic modelling. *Chemical Communications*, **2008**, 214-6	5.8	58
199	Computer modelling of enzyme catalysed reaction mechanisms. *Protein Engineering, Design and Selection*, **1993**, 6, 133-47	1.9	58
198	Teaching Enzyme Catalysis Using Interactive Molecular Dynamics in Virtual Reality. *Journal of Chemical Education*, **2019**, 96, 2488-2496	2.4	56
197	High-Accuracy Computation of Reaction Barriers in Enzymes. *Angewandte Chemie*, **2006**, 118, 7010-7013	3.6	56

196	Determinants of reactivity and selectivity in soluble epoxide hydrolase from quantum mechanics/molecular mechanics modeling. *Biochemistry*, **2012**, 51, 1774-86	3.2	54
195	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
194	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
193	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
192	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
191	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	16.4	52
190	QM/MM modeling of compound I active species in cytochrome P450, cytochrome C peroxidase, and ascorbate peroxidase. *Journal of Computational Chemistry*, **2006**, 27, 1352-62	3.5	51
189	Conformational effects in enzyme catalysis: QM/MM free energy calculation of the 'NAC' contribution in chorismate mutase. *Chemical Communications*, **2004**, 1238-9	5.8	51
188	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
187	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
186	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
185	Tunneling and classical paths for proton transfer in an enzyme reaction dominated by tunneling: oxidation of tryptamine by aromatic amine dehydrogenase. *Journal of Physical Chemistry B*, **2007**, 111, 3032-47	3.4	49
184	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
183	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
182	A Community Letter Regarding Sharing Biomolecular Simulation Data for COVID-19. *Journal of Chemical Information and Modeling*, **2020**, 60, 2653-2656	6.1	45
181	Chemical accuracy in QM/MM calculations on enzyme-catalysed reactions. *Chemistry Central Journal* , **2007**, 1, 19		45
180	Modeling biotransformation reactions by combined quantum mechanical/molecular mechanical approaches: from structure to activity. *Current Topics in Medicinal Chemistry*, **2003**, 3, 1241-56	3	44
179	Large-Scale Density Functional Theory Transition State Searching in Enzymes. *Journal of Physical Chemistry Letters*, **2014**, 5, 3614-9	6.4	43

178	Analysis of polarization in QM/MM modelling of biologically relevant hydrogen bonds. *Journal of the Royal Society Interface*, **2008**, 5 Suppl 3, S207-16	4.1	43
177	Rapid decomposition and visualisation of protein-ligand binding free energies by residue and by water. *Faraday Discussions*, **2014**, 169, 477-99	3.6	42
176	Dynamical origins of heat capacity changes in enzyme-catalysed reactions. *Nature Communications*, **2018**, 9, 1177	17.4	41
175	Computational enzymology: insight into biological catalysts from modelling. *Natural Product Reports*, **2008**, 25, 1001-14	15.1	41
174	Mechanisms of reaction in cytochrome P450: Hydroxylation of camphor in P450cam. *Organic and Biomolecular Chemistry*, **2006**, 4, 3931-7	3.9	41
173	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
172	A multiscale approach to modelling drug metabolism by membrane-bound cytochrome P450 enzymes. *PLoS Computational Biology*, **2014**, 10, e1003714	5	38
171	Combined Quantum and Molecular Mechanical Study of DNA Crosslinking by Nitrous Acid. *Journal of the American Chemical Society*, **1995**, 117, 4706-4707	16.4	38
170	Computational enzymology: modelling the mechanisms of biological catalysts. *Biochemical Society Transactions*, **2008**, 36, 22-6	5.1	37
169	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
168	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
167	High-level QM/MM modelling predicts an arginine as the acid in the condensation reaction catalysed by citrate synthase. *Chemical Communications*, **2008**, 1874-6	5.8	36
166	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
165	Analysis of classical and quantum paths for deprotonation of methylamine by methylamine dehydrogenase. *ChemPhysChem*, **2007**, 8, 1816-35	3.2	35
164	Computational assay of H7N9 influenza neuraminidase reveals R292K mutation reduces drug binding affinity. *Scientific Reports*, **2013**, 3, 3561	4.9	34
163	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 beta-lactamase. *Journal of Physical Chemistry A*, **2009**, 113, 11984-94	2.8	34
162	Insights into the mechanism and inhibition of fatty acid amide hydrolase from quantum mechanics/molecular mechanics (QM/MM) modelling. *Biochemical Society Transactions*, **2009**, 37, 363-7	5.1	34
161	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, 163-75, 214	2.8	34

160	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
159	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
158	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	4.2	33
157	De Novo-Designed □Helical Barrels as Receptors for Small Molecules. *ACS Synthetic Biology*, **2018**, 7, 1808-1816	5.7	33
156	A Photoresponsive Stiff-Stilbene Ligand Fuels the Reversible Unfolding of G-Quadruplex DNA. *Angewandte Chemie - International Edition*, **2019**, 58, 4334-4338	16.4	32
155	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
154	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, 12909-15	3.4	32
153	The Fe-CO bond energy in myoglobin: a QM/MM study of the effect of tertiary structure. *Biophysical Journal*, **2006**, 90, L27-9	2.9	32
152	Modeling Enzyme Reaction Intermediates and Transition States: Citrate Synthase. *Journal of Physical Chemistry B*, **1998**, 102, 6635-6646	3.4	32
151	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
150	QM/MM simulations as an assay for carbapenemase activity in class A □lactamases. *Chemical Communications*, **2014**, 50, 14736-9	5.8	30
149	Conformational change and ligand binding in the aristolochene synthase catalytic cycle. *Biochemistry*, **2013**, 52, 8094-105	3.2	29
148	Substrate polarization in enzyme catalysis: QM/MM analysis of the effect of oxaloacetate polarization on acetyl-CoA enolization in citrate synthase. *Proteins: Structure, Function and Bioinformatics*, **2007**, 69, 521-35	4.2	29
147	QM/MM studies of the electronic structure of the compound I intermediate in cytochrome c peroxidase and ascorbate peroxidase. *Dalton Transactions*, **2005**, 3470-6	4.3	29
146	Biocatalytic Routes to Lactone Monomers for Polymer Production. *Biochemistry*, **2018**, 57, 1997-2008	3.2	28
145	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
144	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
143	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

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141	Computational and experimental studies on the catalytic mechanism of biliverdin-IXbeta reductase. *Biochemical Journal*, **2008**, 411, 475-84	3.8	27
140	Molecular Basis of Class A β-Lactamase Inhibition by Relebactam. *Antimicrobial Agents and Chemotherapy*, **2019**, 63,	5.9	26
139	The QM/MM Approach to Enzymatic Reactions. *Theoretical and Computational Chemistry*, **2001**, 597-653		26
138	Cooperative symmetric to asymmetric conformational transition of the apo-form of scavenger decapping enzyme revealed by simulations. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 498-508	4.2	25
137	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
136	Maintaining and breaking symmetry in homomeric coiled-coil assemblies. *Nature Communications*, **2018**, 9, 4132	17.4	25
135	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
134	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	2.8	24
133	Ab initio QM/MM modelling of acetyl-CoA deprotonation in the enzyme citrate synthase. *Journal of Molecular Graphics and Modelling*, **2007**, 26, 676-90	2.8	23
132	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
131	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
130	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
129	MM and QM/MM Modeling of Threonyl-tRNA Synthetase: Model Testing and Simulations. *Structural Chemistry*, **2004**, 15, 405-414	1.8	22
128	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
127	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
126	QM/MM study on the mechanism of peptide hydrolysis by carboxypeptidase A. *Computational and Theoretical Chemistry*, **2009**, 898, 106-114		21
125	A Multiscale Simulation Approach to Modeling Drug-Protein Binding Kinetics. *Journal of Chemical Theory and Computation*, **2018**, 14, 6093-6101	6.4	21

124	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
123	Unlocking Nicotinic Selectivity via Direct C-H Functionalization of (−)-Cytisine. *CheM*, **2018**, 4, 1710-1725	16.2	20
122	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
121	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
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118	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
117	Mechanistic Insights into the Reaction of Chlorination of Tryptophan Catalyzed by Tryptophan 7-Halogenase. *Scientific Reports*, **2017**, 7, 17395	4.9	19
116	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
115	Modeling protein splicing: reaction pathway for C-terminal splice and intein scission. *Journal of Physical Chemistry B*, **2009**, 113, 5607-16	3.4	19
114	Enzyme evolution and the temperature dependence of enzyme catalysis. *Current Opinion in Structural Biology*, **2020**, 65, 96-101	8.1	18
113	Quantum chemical analysis of reaction paths in chorismate mutase: Conformational effects and electrostatic stabilization. *International Journal of Quantum Chemistry*, **2007**, 107, 2274-2285	2.1	18
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110	A potential interaction between the SARS-CoV-2 spike protein and nicotinic acetylcholine receptors. *Biophysical Journal*, **2021**, 120, 983-993	2.9	18
109	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
108	Interactive molecular dynamics in virtual reality for accurate flexible protein-ligand docking. *PLoS ONE*, **2020**, 15, e0228461	3.7	17
107	Multiscale simulation approaches to modeling drug-protein binding. *Current Opinion in Structural Biology*, **2020**, 61, 213-221	8.1	17

106	Multiscale analysis of enantioselectivity in enzyme-catalysed 'lethal synthesis' using projector-based embedding. *Royal Society Open Science*, **2018**, 5, 171390	3.3	17
105	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
104	"Lethal synthesis" of fluorocitrate by citrate synthase explained through QM/MM modeling. *Angewandte Chemie - International Edition*, **2011**, 50, 10349-51	16.4	17
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101	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
100	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
99	Protein dynamics and enzyme catalysis: the ghost in the machine?. *Biochemical Society Transactions*, **2012**, 40, 515-21	5.1	16
98	A model of the condensation step in the citrate synthase reaction. *Computational and Theoretical Chemistry*, **1998**, 427, 175-184		16
97	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
96	Biomolecular Simulations in the Time of COVID19, and After. *Computing in Science and Engineering*, **2020**, 22, 30-36	1.5	16
95	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
94	Computer simulations of quantum tunnelling in enzyme-catalysed hydrogen transfer reactions. *Interdisciplinary Sciences, Computational Life Sciences*, **2010**, 2, 78-97	3.5	15
93	Cyclic boronates as versatile scaffolds for KPC-2 β-lactamase inhibition. *RSC Medicinal Chemistry*, **2020**, 11, 491-496	3.5	14
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90	Designing better enzymes: Insights from directed evolution. *Current Opinion in Structural Biology*, **2021**, 67, 212-218	8.1	14
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