

JosÃ© Javier Ruiz-PernÃ¡a

List of Publications by Year in descending order

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52
papers

1,324
citations

304368

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58
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58
docs citations

58
times ranked

1190
citing authors

#	ARTICLE	IF	CITATIONS
1	Testing Affordable Strategies for the Computational Study of Reactivity in Cysteine Proteases: The Case of SARS-CoV-2 3CL Protease Inhibition. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4005-4013.	2.3	9
2	Computational simulations on the binding and reactivity of a nitrile inhibitor of the SARS-CoV-2 main protease. <i>Chemical Communications</i> , 2021, 57, 9096-9099.	2.2	32
3	Multiscale Simulations of SARS-CoV-2 3CL Protease Inhibition with Aldehyde Derivatives. Role of Protein and Inhibitor Conformational Changes in the Reaction Mechanism. <i>ACS Catalysis</i> , 2021, 11, 4157-4168.	5.5	40
4	Mechanistic study of the biosynthesis of R-phenylcarbinol by acetohydroxyacid synthase enzyme using hybrid quantum mechanics/molecular mechanics simulations. <i>Archives of Biochemistry and Biophysics</i> , 2021, 701, 108807.	1.4	1
5	Corrigendum to "Mechanistic study of the biosynthesis of R-phenylacetylcarbinol by acetohydroxyacid synthase enzyme using hybrid quantum mechanics/molecular mechanics simulations" [Arch. Biochem. Biophys. 701 (2021) 108807]. <i>Archives of Biochemistry and Biophysics</i> , 2021, 707, 108848.	1.4	0
6	Inhibition Mechanism of SARS-CoV-2 Main Protease with Ketone-Based Inhibitors Unveiled by Multiscale Simulations: Insights for Improved Designs**. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 25933-25941.	7.2	24
7	A microscopic description of SARS-CoV-2 main protease inhibition with Michael acceptors. Strategies for improving inhibitor design. <i>Chemical Science</i> , 2021, 12, 3489-3496.	3.7	40
8	Computational Insights Into Enzyme Catalysis. , 2020, , 560-577.		0
9	On the Nature of the Enzyme-Substrate Complex and the Reaction Mechanism in Human Arginase I. A Combined Molecular Dynamics and QM/MM Study. <i>ACS Catalysis</i> , 2020, 10, 8321-8333.	5.5	9
10	Unraveling the SARS-CoV-2 Main Protease Mechanism Using Multiscale Methods. <i>ACS Catalysis</i> , 2020, 10, 12544-12554.	5.5	107
11	Loss of Hyperconjugative Effects Drives Hydride Transfer during Dihydrofolate Reductase Catalysis. <i>ACS Catalysis</i> , 2019, 9, 10343-10349.	5.5	1
12	Why Are Some Enzymes Dimers? Flexibility and Catalysis in <i>Thermotoga maritima</i> Dihydrofolate Reductase. <i>ACS Catalysis</i> , 2019, 9, 5902-5911.	5.5	12
13	Translocation of Enzymes into a Mesoporous MOF for Enhanced Catalytic Activity Under Extreme Conditions. <i>Chemical Science</i> , 2019, 10, 4082-4088.	3.7	47
14	A molecular dynamics study on the role of the protonation state in the biosynthesis of R-PAC by AHAS. <i>Chemical Physics Letters</i> , 2019, 716, 247-251.	1.2	4
15	Isotope Substitution of Promiscuous Alcohol Dehydrogenase Reveals the Origin of Substrate Preference in the Transition State. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 3128-3131.	7.2	10
16	Temperature dependence of dynamic, tunnelling and kinetic isotope effects in formate dehydrogenase. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25722-25737.	1.3	2
17	Isotope Substitution of Promiscuous Alcohol Dehydrogenase Reveals the Origin of Substrate Preference in the Transition State. <i>Angewandte Chemie</i> , 2018, 130, 3182-3185.	1.6	2
18	QM/MM study of lactate oxidation by flavocytochrome b ₂ . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15609-15618.	1.3	10

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19	Minimization of dynamic effects in the evolution of dihydrofolate reductase. <i>Chemical Science</i> , 2016, 7, 3248-3255.	3.7	25
20	Chemical Ligation and Isotope Labeling to Locate Dynamic Effects during Catalysis by Dihydrofolate Reductase. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 9016-9020.	7.2	35
21	Tuning the Phosphoryl Donor Specificity of Dihydroxyacetone Kinase from ATP to Inorganic Polyphosphate. An Insight from Computational Studies. <i>International Journal of Molecular Sciences</i> , 2015, 16, 27835-27849.	1.8	11
22	A computational study of the phosphoryl transfer reaction between ATP and Dha in aqueous solution. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 10179-10190.	1.5	4
23	Linking Electrostatic Effects and Protein Motions in Enzymatic Catalysis. A Theoretical Analysis of Catechol <i>O</i> -Methyltransferase. <i>Journal of Physical Chemistry B</i> , 2015, 119, 873-882.	1.2	14
24	Exploring Chemical Reactivity in Enzyme Catalyzed Processes Using QM/MM Methods: An Application to Dihydrofolate Reductase. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 383-413.	0.6	1
25	Protein Isotope Effects in Dihydrofolate Reductase From <i>Geobacillus stearothermophilus</i> Show Entropic-Enthalpic Compensatory Effects on the Rate Constant. <i>Journal of the American Chemical Society</i> , 2014, 136, 17317-17323.	6.6	34
26	Heavy enzymes- experimental and computational insights in enzyme dynamics. <i>Current Opinion in Chemical Biology</i> , 2014, 21, 11-18.	2.8	39
27	QM/MM kinetic isotope effects for chloromethane hydrolysis in water. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 1058-1065.	0.9	3
28	Toward an Automatic Determination of Enzymatic Reaction Mechanisms and Their Activation Free Energies. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3740-3749.	2.3	37
29	Studying the role of protein dynamics in an SN2 enzyme reaction using free-energy surfaces and solvent coordinates. <i>Nature Chemistry</i> , 2013, 5, 566-571.	6.6	49
30	Increased Dynamic Effects in a Catalytically Compromised Variant of <i>Escherichia coli</i> Dihydrofolate Reductase. <i>Journal of the American Chemical Society</i> , 2013, 135, 18689-18696.	6.6	56
31	Unraveling the role of protein dynamics in dihydrofolate reductase catalysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 16344-16349.	3.3	119
32	A Novel Strategy to Study Electrostatic Effects in Chemical Reactions: Differences between the Role of Solvent and the Active Site of Chalcone Isomerase in a Michael Addition. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1532-1535.	2.3	10
33	Hydrolysis of Phosphotriesters: A Theoretical Analysis of the Enzymatic and Solution Mechanisms. <i>Chemistry - A European Journal</i> , 2012, 18, 9612-9621.	1.7	26
34	Ensemble-Averaged QM/MM Kinetic Isotope Effects for the S _N 2 Reaction of Cyanide Anions with Chloroethane in DMSO Solution. <i>Chemistry - A European Journal</i> , 2012, 18, 9405-9414.	1.7	13
35	Hybrid Schemes Based on Quantum Mechanics/Molecular Mechanics Simulations. <i>Advances in Protein Chemistry and Structural Biology</i> , 2011, 85, 81-142.	1.0	19
36	Does glycosyl transfer involve an oxacarbenium intermediate? Computational simulation of the lifetime of the methoxymethyl cation in water. <i>Pure and Applied Chemistry</i> , 2011, 83, 1507-1514.	0.9	9

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37	Computational Simulation of the Lifetime of the Methoxymethyl Cation in Water. A Simple Model for a Glycosyl Cation: When Is an Intermediate an Intermediate?. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5769-5774.	1.2	11
38	A QM/MM study of the reaction mechanism for the 3' processing step catalyzed by HIV-1 integrase. <i>Computational and Theoretical Chemistry</i> , 2009, 898, 115-120.	1.5	8
39	Theoretical Modeling on the Reaction Mechanism of p-Nitrophenylmethylphosphate Alkaline Hydrolysis and its Kinetic Isotope Effects. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 439-442.	2.3	16
40	Critical Role of Substrate Conformational Change in the Proton Transfer Process Catalyzed by 4-Oxalocrotonate Tautomerase. <i>Journal of the American Chemical Society</i> , 2009, 131, 2687-2698.	6.6	18
41	Computational mutagenesis reveals the role of active-site tyrosine in stabilising a boat conformation for the substrate: QM/MM molecular dynamics studies of wild-type and mutant xylanases. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 460-468.	1.5	36
42	Mechanism of glycoside hydrolysis: A comparative QM/MM molecular dynamics analysis for wild type and Y69F mutant retaining xylanases. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 5236.	1.5	28
43	Dynamic Effects on Reaction Rates in a Michael Addition Catalyzed by Chalcone Isomerase. Beyond the Frozen Environment Approach. <i>Journal of the American Chemical Society</i> , 2008, 130, 7477-7488.	6.6	61
44	QM/MM simulations for methyl transfer in solution and catalysed by COMT: ensemble-averaging of kinetic isotope effects. <i>Chemical Communications</i> , 2008, , 6114.	2.2	25
45	Analysis of the Decarboxylation Step in Mammalian Histidine Decarboxylase. <i>Journal of Biological Chemistry</i> , 2008, 283, 12393-12401.	1.6	24
46	Enzymatic Effects on Reactant and Transition States. The Case of Chalcone Isomerase. <i>Journal of the American Chemical Society</i> , 2007, 129, 9117-9124.	6.6	16
47	Hybrid Quantum Mechanics/Molecular Mechanics Simulations with Two-Dimensional Interpolated Corrections: An Application to Enzymatic Processes. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17663-17670.	1.2	57
48	Activation Free Energy of Catechol O-Methyltransferase. Corrections to the Potential of Mean Force. <i>Journal of Physical Chemistry A</i> , 2006, 110, 503-509.	1.1	32
49	Comparative Computational Analysis of Different Active Site Conformations and Substrates in a Chalcone Isomerase Catalyzed Reaction. <i>Journal of Physical Chemistry B</i> , 2006, 110, 20686-20692.	1.2	15
50	A QM/MM Exploration of the Potential Energy Surface of Pyruvate to Lactate Transformation Catalyzed by LDH. Improving the Accuracy of Semiempirical Descriptions. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 750-761.	2.3	22
51	Hybrid QM/MM Potentials of Mean Force with Interpolated Corrections. <i>Journal of Physical Chemistry B</i> , 2004, 108, 8427-8433.	1.2	95
52	Inhibition Mechanism of SARS-CoV-2 Main Protease with Ketone-Based Inhibitors Unveiled by Multiscale Simulations. Insights for Improved Designs. <i>Angewandte Chemie</i> , 0, , .	1.6	0