JosÃ© Javier Ruiz-PernÃ-a

List of Publications by Year
in descending order

52	1,324	304602	360920
papers	citations	22 h-index	35 g-index

58	58	58	1190
all docs	docs citations	times ranked	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. Journal of Chemical Theory and Computation, 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. Chemical Communications, 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. ACS Catalysis, 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. Archives of Biochemistry and Biophysics, 2021, 701, 108807.	1.4	1
5	Corrigendum to â€œMechanistic study of the biosynthesis of R-phenylacetylcarbinol by acetohydroxyacid synthase enzyme using hybrid quantum mechanics/molecular mechanics simulationsâ€•[Arch. Biochem. Biophys. 701 (2021) 108807]. Archives of Biochemistry and Biophysics, 2021, 707, 108848.	1.4	0
6	Inhibition Mechanism of SARSâ€CoVâ€2 Main Protease with Ketoneâ€Based Inhibitors Unveiled by Multiscale Simulations: Insights for Improved Designs**. Angewandte Chemie - International Edition, 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. Chemical Science, 2021, 12, 3489-3496.	3.7	40
8	Computational Insights Into Enzyme Catalysis. , 2020, , 560-577.		0
9	On the Nature of the Enzymeâ€“Substrate Complex and the Reaction Mechanism in Human Arginase I. A Combined Molecular Dynamics and QM/MM Study. ACS Catalysis, 2020, 10, 8321-8333.	5.5	9
10	Unraveling the SARS-CoV-2 Main Protease Mechanism Using Multiscale Methods. ACS Catalysis, 2020, 10, 12544-12554.	5.5	107
11	Loss of Hyperconjugative Effects Drives Hydride Transfer during Dihydrofolate Reductase Catalysis. ACS Catalysis, 2019, 9, 10343-10349.	5.5	1
12	Why Are Some Enzymes Dimers? Flexibility and Catalysis in Thermotoga maritima Dihydrofolate Reductase. ACS Catalysis, 2019, 9, 5902-5911.	5.5	12
13	Translocation of Enzymes into a Mesoporous MOF for Enhanced Catalytic Activity Under Extreme Conditions. Chemical Science, 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. Chemical Physics Letters, 2019, 716, 247-251.	1.2	4
15	Isotope Substitution of Promiscuous Alcohol Dehydrogenase Reveals the Origin of Substrate Preference in the Transition State. Angewandte Chemie - International Edition, 2018, 57, 3128-3131.	7.2	10
16	Temperature dependence of dynamic, tunnelling and kinetic isotope effects in formate dehydrogenase. Physical Chemistry Chemical Physics, 2018, 20, 25722-25737.	1.3	2
17	Isotope Substitution of Promiscuous Alcohol Dehydrogenase Reveals the Origin of Substrate Preference in the Transition State. Angewandte Chemie, 2018, 130, 3182-3185.	1.6	2
18	QM/MM study of<scp>l</scp>-lactate oxidation by flavocytochrome b₂. Physical Chemistry Chemical Physics, 2016, 18, 15609-15618.	1.3	10

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19	Minimization of dynamic effects in the evolution of dihydrofolate reductase. Chemical Science, 2016, 7, 3248-3255.	3.7	25
20	Chemical Ligation and Isotope Labeling to Locate Dynamic Effects during Catalysis by Dihydrofolate Reductase. Angewandte Chemie - International Edition, 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. International Journal of Molecular Sciences, 2015, 16, 27835-27849.	1.8	11
22	A computational study of the phosphoryl transfer reaction between ATP and Dha in aqueous solution. Organic and Biomolecular Chemistry, 2015, 13, 10179-10190.	1.5	4
23	Linking Electrostatic Effects and Protein Motions in Enzymatic Catalysis. A Theoretical Analysis of Catechol O-Methyltransferase. Journal of Physical Chemistry B, 2015, 119, 873-882.	1.2	14
24	Exploring Chemical Reactivity in Enzyme Catalyzed Processes Using QM/MM Methods: An Application to Dihydrofolate Reductase. Challenges and Advances in Computational Chemistry and Physics, 2015, , 383-413.	0.6	1
25	Protein Isotope Effects in Dihydrofolate Reductase From Geobacillus stearothermophilus Show Entropicâ€“Enthalpic Compensatory Effects on the Rate Constant. Journal of the American Chemical Society, 2014, 136, 17317-17323.	6.6	34
26	Heavy enzymesâ€”experimental and computational insights in enzyme dynamics. Current Opinion in Chemical Biology, 2014, 21, 11-18.	2.8	39
27	QM/MM kinetic isotope effects for chloromethane hydrolysis in water. Journal of Physical Organic Chemistry, 2013, 26, 1058-1065.	0.9	3
28	Toward an Automatic Determination of Enzymatic Reaction Mechanisms and Their Activation Free Energies. Journal of Chemical Theory and Computation, 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. Nature Chemistry, 2013, 5, 566-571.	6.6	49
30	Increased Dynamic Effects in a Catalytically Compromised Variant of Escherichia coli Dihydrofolate Reductase. Journal of the American Chemical Society, 2013, 135, 18689-18696.	6.6	56
31	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
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. Journal of Chemical Theory and Computation, 2012, 8, 1532-1535.	2.3	10
33	Hydrolysis of Phosphotriesters: A Theoretical Analysis of the Enzymatic and Solution Mechanisms. Chemistry - A European Journal, 2012, 18, 9612-9621.	1.7	26
34	Ensembleâ€Averaged QM/MM Kinetic Isotope Effects for the S_N2 Reaction of Cyanide Anions with Chloroethane in DMSO Solution. Chemistry - A European Journal, 2012, 18, 9405-9414.	1.7	13
35	Hybrid Schemes Based on Quantum Mechanics/Molecular Mechanics Simulations. Advances in Protein Chemistry and Structural Biology, 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. Pure and Applied Chemistry, 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?. Journal of Physical Chemistry B, 2010, 114, 5769-5774.	1.2	11
38	A QM/MM study of the reaction mechanism for the 3â€²-processing step catalyzed by HIV-1 integrase. Computational and Theoretical Chemistry, 2009, 898, 115-120.	1.5	8
39	Theoretical Modeling on the Reaction Mechanism of p-Nitrophenylmethylphosphate Alkaline Hydrolysis and its Kinetic Isotope Effects. Journal of Chemical Theory and Computation, 2009, 5, 439-442.	2.3	16
40	Critical Role of Substrate Conformational Change in the Proton Transfer Process Catalyzed by 4-Oxalocrotonate Tautomerase. Journal of the American Chemical Society, 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. Organic and Biomolecular Chemistry, 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. Organic and Biomolecular Chemistry, 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. Journal of the American Chemical Society, 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. Chemical Communications, 2008, , 6114.	2.2	25
45	Analysis of the Decarboxylation Step in Mammalian Histidine Decarboxylase. Journal of Biological Chemistry, 2008, 283, 12393-12401.	1.6	24
46	Enzymatic Effects on Reactant and Transition States. The Case of Chalcone Isomerase. Journal of the American Chemical Society, 2007, 129, 9117-9124.	6.6	16
47	Hybrid Quantum Mechanics/Molecular Mechanics Simulations with Two-Dimensional Interpolated Corrections:Â Application to Enzymatic Processes. Journal of Physical Chemistry B, 2006, 110, 17663-17670.	1.2	57
48	Activation Free Energy of CatecholO-Methyltransferase. Corrections to the Potential of Mean Forceâ€. Journal of Physical Chemistry A, 2006, 110, 503-509.	1.1	32
49	Comparative Computational Analysis of Different Active Site Conformations and Substrates in a Chalcone Isomerase Catalyzed Reaction. Journal of Physical Chemistry B, 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. Journal of Chemical Theory and Computation, 2005, 1, 750-761.	2.3	22
51	Hybrid QM/MM Potentials of Mean Force with Interpolated Corrections. Journal of Physical Chemistry B, 2004, 108, 8427-8433.	1.2	95
52	Inhibition Mechanism of SARSâ€CoVâ€2 Main Protease with Ketoneâ€Based Inhibitors Unveiled by Multiscale Simulations. Insights for Improved Designs. Angewandte Chemie, 0, , .	1.6	0