

Maite Roca

List of Publications by Year in descending order

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papers

1,386
citations

394286

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39
all docs

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docs citations

39
times ranked

1399
citing authors

#	ARTICLE	IF	CITATIONS
1	Unrevealing the Proteolytic Activity of RgpB Gingipain from Computational Simulations. Journal of Chemical Information and Modeling, 2021, 61, 4582-4593.	2.5	4
2	Elucidating the Catalytic Reaction Mechanism of Orotate Phosphoribosyltransferase by Means of X-ray Crystallography and Computational Simulations. ACS Catalysis, 2020, 10, 1871-1885.	5.5	9
3	Selective oxidation of alkyl and aryl glyceryl monoethers catalysed by an engineered and immobilised glycerol dehydrogenase. Chemical Science, 2020, 11, 12009-12020.	3.7	9
4	Critical evaluation of anharmonicity and configurational averaging in QM/MM modelling of equilibrium isotope effects. Physical Chemistry Chemical Physics, 2020, 22, 16267-16276.	1.3	3
5	Transition-State Vibrational Analysis and Isotope Effects for COMT-Catalyzed Methyl Transfer. Journal of the American Chemical Society, 2020, 142, 15548-15559.	6.6	3
6	Origin of Enzymatic Kinetic Isotope Effects in Human Purine Nucleoside Phosphorylase. ACS Catalysis, 2018, 8, 815-827.	5.5	5
7	Temperature dependence of dynamic, tunnelling and kinetic isotope effects in formate dehydrogenase. Physical Chemistry Chemical Physics, 2018, 20, 25722-25737.	1.3	2
8	Unraveling the Reaction Mechanism of Enzymatic C5-Cytosine Methylation of DNA. A Combined Molecular Dynamics and QM/MM Study of Wild Type and Gln119 Variant. ACS Catalysis, 2016, 6, 3262-3276.	5.5	30
9	Enzyme Promiscuity in Enolase Superfamily. Theoretical Study of <i>Succinylbenzoate Synthase</i> Using QM/MM Methods. Journal of Physical Chemistry B, 2015, 119, 1899-1911.	1.2	6
10	Linking Electrostatic Effects and Protein Motions in Enzymatic Catalysis. A Theoretical Analysis of Catechol <i>O</i> -Methyltransferase. Journal of Physical Chemistry B, 2015, 119, 873-882.	1.2	14
11	Dynamics and Reactivity in <i>Thermus aquaticus</i> N6-Adenine Methyltransferase. Journal of the American Chemical Society, 2014, 136, 16227-16239.	6.6	22
12	The Catalytic Mechanism of Carboxylesterases: A Computational Study. Biochemistry, 2014, 53, 5820-5829.	1.2	53
13	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
14	Modeling methods for studying post-translational and transcriptional modifying enzymes. Current Opinion in Chemical Biology, 2012, 16, 465-471.	2.8	5
15	Substrate promiscuity in DNA methyltransferase M.PvuII. A mechanistic insight. Organic and Biomolecular Chemistry, 2012, 10, 5395.	1.5	8
16	Reversibility and Diffusion in Mandelythiamin Decarboxylation. Searching Dynamical Effects in Decarboxylation Reactions. Journal of the American Chemical Society, 2012, 134, 10509-10514.	6.6	8
17	Promiscuity in Alkaline Phosphatase Superfamily. Unraveling Evolution through Molecular Simulations. Journal of the American Chemical Society, 2011, 133, 12050-12062.	6.6	61
18	Do Dynamic Effects Play a Significant Role in Enzymatic Catalysis? A Theoretical Analysis of Formate Dehydrogenase. Chemistry - A European Journal, 2010, 16, 11399-11411.	1.7	25

#	ARTICLE	IF	CITATIONS
19	Multiscale simulations of protein landscapes: Using coarse-grained models as reference potentials to full explicit models. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1212-1227.	1.5	62
20	Application of Grote-Hynes Theory to the Reaction Catalyzed by Thymidylate Synthase. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13593-13600.	1.2	17
21	Theoretical Study of Phosphodiester Hydrolysis in Nucleotide Pyrophosphatase/Phosphodiesterase. Environmental Effects on the Reaction Mechanism. <i>Journal of the American Chemical Society</i> , 2010, 132, 6955-6963.	6.6	51
22	Theoretical Study of the Catalytic Mechanism of DNA-(N4-Cytosine)-Methyltransferase from the Bacterium <i>Proteus vulgaris</i> . <i>Journal of Physical Chemistry B</i> , 2010, 114, 8467-8473.	1.2	10
23	Theoretical study of the temperature dependence of dynamic effects in thymidylate synthase. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11657.	1.3	15
24	Effective approach for calculations of absolute stability of proteins using focused dielectric constants. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 77, 670-684.	1.5	62
25	The empirical valence bond as an effective strategy for computer-aided enzyme design. <i>Biotechnology Journal</i> , 2009, 4, 495-500.	1.8	11
26	Toward Accurate Screening in Computer-Aided Enzyme Design. <i>Biochemistry</i> , 2009, 48, 3046-3056.	1.2	62
27	Coupling of the guanosine glycosidic bond conformation and the ribonucleotide cleavage reaction: Implications for barnase catalysis. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 415-428.	1.5	2
28	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
29	Using Grote-Hynes Theory To Quantify Dynamical Effects on the Reaction Rate of Enzymatic Processes. The Case of Methyltransferases. <i>Journal of Physical Chemistry B</i> , 2008, 112, 529-534.	1.2	17
30	On the relationship between folding and chemical landscapes in enzyme catalysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 13877-13882.	3.3	82
31	Electrostatic contributions to protein stability and folding energy. <i>FEBS Letters</i> , 2007, 581, 2065-2071.	1.3	51
32	On the Relationship between Thermal Stability and Catalytic Power of Enzymes. <i>Biochemistry</i> , 2007, 46, 15076-15088.	1.2	85
33	Coupling between Protein and Reaction Dynamics in Enzymatic Processes: Application of Grote-Hynes Theory to CatecholO-Methyltransferase. <i>Journal of the American Chemical Society</i> , 2006, 128, 6186-6193.	6.6	57
34	Activation Free Energy of CatecholO-Methyltransferase. Corrections to the Potential of Mean Force. <i>Journal of Physical Chemistry A</i> , 2006, 110, 503-509.	1.1	32
35	On the Nature of the Transition State in CatecholO-Methyltransferase. A Complementary Study Based on Molecular Dynamics and Potential Energy Surface Explorations. <i>Journal of the American Chemical Society</i> , 2005, 127, 10648-10655.	6.6	43
36	Theoretical Insights in Enzyme Catalysis. <i>ChemInform</i> , 2004, 35, no.	0.1	0

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37	QM/MM Determination of Kinetic Isotope Effects for COMT-Catalyzed Methyl Transfer Does Not Support Compression Hypothesis. <i>Journal of the American Chemical Society</i> , 2004, 126, 8634-8635.	6.6	51
38	Theoretical insights in enzyme catalysis. <i>Chemical Society Reviews</i> , 2004, 33, 98-107.	18.7	150
39	Theoretical Modeling of Enzyme Catalytic Power:Â Analysis of â€œCraticâ€ and Electrostatic Factors in CatecholO-Methyltransferase. <i>Journal of the American Chemical Society</i> , 2003, 125, 7726-7737.	6.6	79