Maite Roca

List of Publications by Year
in descending order

39 papers	1,386 citations	448610 19 h-index	371746 37 g-index
39 all docs	39 docs citations	39 times ranked	1585 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 o-Succinylbenzoate Synthase 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 O-Methyltransferase. Journal of Physical Chemistry B, 2015, 119, 873-882.	1.2	14
11	Dynamics and Reactivity in Thermus aquaticus 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 coarseâ€grained models as reference potentials to full explicit models. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1212-1227.	1.5	62
20	Application of Groteâ€™Hynes Theory to the Reaction Catalyzed by Thymidylate Synthase. Journal of Physical Chemistry B, 2010, 114, 13593-13600.	1.2	17
21	Theoretical Study of Phosphodiester Hydrolysis in Nucleotide Pyrophosphatase/Phosphodiesterase. Environmental Effects on the Reaction Mechanism. Journal of the American Chemical Society, 2010, 132, 6955-6963.	6.6	51
22	Theoretical Study of the Catalytic Mechanism of DNA-(N4-Cytosine)-Methyltransferase from the Bacterium Proteus vulgaris. Journal of Physical Chemistry B, 2010, 114, 8467-8473.	1.2	10
23	Theoretical study of the temperature dependence of dynamic effects in thymidylate synthase. Physical Chemistry Chemical Physics, 2010, 12, 11657.	1.3	15
24	Effective approach for calculations of absolute stability of proteins using focused dielectric constants. Proteins: Structure, Function and Bioinformatics, 2009, 77, 670-684.	1.5	62
25	The empirical valence bond as an effective strategy for computerâ€aided enzyme design. Biotechnology Journal, 2009, 4, 495-500.	1.8	11
26	Toward Accurate Screening in Computer-Aided Enzyme Design. Biochemistry, 2009, 48, 3046-3056.	1.2	62
27	Coupling of the guanosine glycosidic bond conformation and the ribonucleotide cleavage reaction: Implications for barnase catalysis. Proteins: Structure, Function and Bioinformatics, 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. Journal of the American Chemical Society, 2008, 130, 7477-7488.	6.6	61
29	Using Groteâ€™Hynes Theory To Quantify Dynamical Effects on the Reaction Rate of Enzymatic Processes. The Case of Methyltransferases. Journal of Physical Chemistry B, 2008, 112, 529-534.	1.2	17
30	On the relationship between folding and chemical landscapes in enzyme catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 13877-13882.	3.3	82
31	Electrostatic contributions to protein stability and folding energy. FEBS Letters, 2007, 581, 2065-2071.	1.3	51
32	On the Relationship between Thermal Stability and Catalytic Power of Enzymes. Biochemistry, 2007, 46, 15076-15088.	1.2	85
33	Coupling between Protein and Reaction Dynamics in Enzymatic Processes:Â Application of Groteâ€™Hynes Theory to CatecholO-Methyltransferase. Journal of the American Chemical Society, 2006, 128, 6186-6193.	6.6	57
34	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
35	On the Nature of the Transition State in CatecholO-Methyltransferase. A Complementary Study Based on Molecular Dynamics and Potential Energy Surface Explorations. Journal of the American Chemical Society, 2005, 127, 10648-10655.	6.6	43
36	Theoretical Insights in Enzyme Catalysis. ChemInform, 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. Journal of the American Chemical Society, 2004, 126, 8634-8635.	6.6	51
38	Theoretical insights in enzyme catalysis. Chemical Society Reviews, 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. Journal of the American Chemical Society, 2003, 125, 7726-7737.	6.6	79