

# Maite Roca

## List of Publications by Year in descending order

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39  
papers

1,386  
citations

394421

19  
h-index

330143

37  
g-index

39  
all docs

39  
docs citations

39  
times ranked

1399  
citing authors

#	ARTICLE	IF	CITATIONS
1	Theoretical insights in enzyme catalysis. <i>Chemical Society Reviews</i> , 2004, 33, 98-107.	38.1	150
2	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.	7.1	119
3	On the Relationship between Thermal Stability and Catalytic Power of Enzymes. <i>Biochemistry</i> , 2007, 46, 15076-15088.	2.5	85
4	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.	7.1	82
5	Theoretical Modeling of Enzyme Catalytic Power: A Analysis of Electrostatic and Electrostatic Factors in CatecholO-Methyltransferase. <i>Journal of the American Chemical Society</i> , 2003, 125, 7726-7737.	13.7	79
6	Effective approach for calculations of absolute stability of proteins using focused dielectric constants. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 77, 670-684.	2.6	62
7	Toward Accurate Screening in Computer-Aided Enzyme Design. <i>Biochemistry</i> , 2009, 48, 3046-3056.	2.5	62
8	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.	2.6	62
9	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.	13.7	61
10	Promiscuity in Alkaline Phosphatase Superfamily. Unraveling Evolution through Molecular Simulations. <i>Journal of the American Chemical Society</i> , 2011, 133, 12050-12062.	13.7	61
11	Coupling between Protein and Reaction Dynamics in Enzymatic Processes: A Application of Grote-Hynes Theory to CatecholO-Methyltransferase. <i>Journal of the American Chemical Society</i> , 2006, 128, 6186-6193.	13.7	57
12	The Catalytic Mechanism of Carboxylesterases: A Computational Study. <i>Biochemistry</i> , 2014, 53, 5820-5829.	2.5	53
13	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.	13.7	51
14	Electrostatic contributions to protein stability and folding energy. <i>FEBS Letters</i> , 2007, 581, 2065-2071.	2.8	51
15	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.	13.7	51
16	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.	13.7	43
17	Activation Free Energy of CatecholO-Methyltransferase. Corrections to the Potential of Mean Force. <i>Journal of Physical Chemistry A</i> , 2006, 110, 503-509.	2.5	32
18	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. <i>ACS Catalysis</i> , 2016, 6, 3262-3276.	11.2	30

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19	Do Dynamic Effects Play a Significant Role in Enzymatic Catalysis? A Theoretical Analysis of Formate Dehydrogenase. <i>Chemistry - A European Journal</i> , 2010, 16, 11399-11411.	3.3	25
20	Dynamics and Reactivity in <i>Thermus aquaticus</i> N6-Adenine Methyltransferase. <i>Journal of the American Chemical Society</i> , 2014, 136, 16227-16239.	13.7	22
21	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.	2.6	17
22	Application of Grote-Hynes Theory to the Reaction Catalyzed by Thymidylate Synthase. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13593-13600.	2.6	17
23	Theoretical study of the temperature dependence of dynamic effects in thymidylate synthase. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11657.	2.8	15
24	Linking Electrostatic Effects and Protein Motions in Enzymatic Catalysis. A Theoretical Analysis of Catechol O-Methyltransferase. <i>Journal of Physical Chemistry B</i> , 2015, 119, 873-882.	2.6	14
25	The empirical valence bond as an effective strategy for computer-aided enzyme design. <i>Biotechnology Journal</i> , 2009, 4, 495-500.	3.5	11
26	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.	2.6	10
27	Elucidating the Catalytic Reaction Mechanism of Orotate Phosphoribosyltransferase by Means of X-ray Crystallography and Computational Simulations. <i>ACS Catalysis</i> , 2020, 10, 1871-1885.	11.2	9
28	Selective oxidation of alkyl and aryl glyceryl monoethers catalysed by an engineered and immobilised glycerol dehydrogenase. <i>Chemical Science</i> , 2020, 11, 12009-12020.	7.4	9
29	Substrate promiscuity in DNA methyltransferase M.PvuII. A mechanistic insight. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 5395.	2.8	8
30	Reversibility and Diffusion in Mandelythiamin Decarboxylation. Searching Dynamical Effects in Decarboxylation Reactions. <i>Journal of the American Chemical Society</i> , 2012, 134, 10509-10514.	13.7	8
31	Enzyme Promiscuity in Enolase Superfamily. Theoretical Study of <i>o</i> -Succinylbenzoate Synthase Using QM/MM Methods. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1899-1911.	2.6	6
32	Modeling methods for studying post-translational and transcriptional modifying enzymes. <i>Current Opinion in Chemical Biology</i> , 2012, 16, 465-471.	6.1	5
33	Origin of Enzymatic Kinetic Isotope Effects in Human Purine Nucleoside Phosphorylase. <i>ACS Catalysis</i> , 2018, 8, 815-827.	11.2	5
34	Unrevealing the Proteolytic Activity of RgpB Gingipain from Computational Simulations. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4582-4593.	5.4	4
35	Critical evaluation of anharmonicity and configurational averaging in QM/MM modelling of equilibrium isotope effects. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16267-16276.	2.8	3
36	Transition-State Vibrational Analysis and Isotope Effects for COMT-Catalyzed Methyl Transfer. <i>Journal of the American Chemical Society</i> , 2020, 142, 15548-15559.	13.7	3

#	ARTICLE	IF	CITATIONS
37	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.	2.6	2
38	Temperature dependence of dynamic, tunnelling and kinetic isotope effects in formate dehydrogenase. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25722-25737.	2.8	2
39	Theoretical Insights in Enzyme Catalysis. <i>ChemInform</i> , 2004, 35, no.	0.0	0