Sergio MartÃ-

List of Publications by Year
in descending order

80 papers	2,275 citations	185998 28 h-index	243296 44 g-index
82 all docs	82 docs citations	82 times ranked	1912 citing authors

#	Article	IF	Citations
1	Impact of Warhead Modulations on the Covalent Inhibition of SARS-CoV-2 M^{pro} Explored by QM/MM Simulations. ACS Catalysis, 2022, 12, 698-708.	5.5	17
2	<scp>QMCube</scp> (<scp>QM³</scp>): An allâ€purpose suite for multiscale <scp>QM</scp>/<scp>MM</scp> calculations. Journal of Computational Chemistry, 2021, 42, 447-457.	1.5	8
3	A QM/MM study on the origin of retro-aldolase activity of a catalytic antibody. Chemical Communications, 2021, 57, 5306-5309.	2.2	0
4	Unrevealing the Proteolytic Activity of RgpB Gingipain from Computational Simulations. Journal of Chemical Information and Modeling, 2021, 61, 4582-4593.	2.5	4
5	Are Heme-Dependent Enzymes Always Using a Redox Mechanism? A Theoretical Study of the Kemp Elimination Catalyzed by a Promiscuous Aldoxime Dehydratase. ACS Catalysis, 2020, 10, 11110-11119.	5.5	7
6	Understanding the Directed Evolution of De Novo Retro-Aldolases from QM/MM Studies. ACS Catalysis, 2020, 10, 7871-7883.	5.5	6
7	Examination of the performance of semiempirical methods in QM/MM studies of the SN2-like reaction of an adenylyl group transfer catalysed by ANT4â€². Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	1
8	QM/MM Theoretical Studies of a de Novo Retro-Aldolase Design. ACS Catalysis, 2019, 9, 2482-2492.	5.5	16
9	Theoretical Studies on Mechanism of Inactivation of Kanamycin A by 4â€²-O-Nucleotidyltransferase. Frontiers in Chemistry, 2018, 6, 660.	1.8	10
10	Molecular mechanism of the site-specific self-cleavage of the RNA phosphodiester backbone by a twister ribozyme. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	6
11	Theoretical Study of the Mechanism of Exemestane Hydroxylation Catalyzed by Human Aromatase Enzyme. Journal of Physical Chemistry B, 2016, 120, 3331-3343.	1.2	5
12	QM/MM modeling of the hydroxylation of the androstenedione substrate catalyzed by cytochrome P450 aromatase (CYP19A1). Journal of Computational Chemistry, 2015, 36, 1736-1747.	1.5	8
13	Protein Conformational Landscapes and Catalysis. Influence of Active Site Conformations in the Reaction Catalyzed by L-Lactate Dehydrogenase. ACS Catalysis, 2015, 5, 1172-1185.	5.5	48
14	Joint Use of Bonding Evolution Theory and QM/MM Hybrid Method for Understanding the Hydrogen Abstraction Mechanism via Cytochrome P450 Aromatase. Journal of Chemical Theory and Computation, 2015, 11, 1470-1480.	2.3	17
15	Peptide Bond Formation Mechanism Catalyzed by Ribosome. Journal of the American Chemical Society, 2015, 137, 12024-12034.	6.6	34
16	Quantum Mechanics/Molecular Mechanics Studies of the Mechanism of Falcipain-2 Inhibition by the Epoxysuccinate E64. Biochemistry, 2014, 53, 3336-3346.	1.2	18
17	Theoretical Study of Primary Reaction of Pseudozyma antarctica Lipase B as the Starting Point To Understand Its Promiscuity. ACS Catalysis, 2014, 4, 426-434.	5.5	31
18	Computational study of the mechanism of half-reactions in class 1A dihydroorotate dehydrogenase from Trypanosoma cruzi. Physical Chemistry Chemical Physics, 2013, 15, 18863.	1.3	7

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19	The catalytic mechanism of glyceraldehyde 3-phosphate dehydrogenase from Trypanosoma cruzi elucidated via the QM/MM approach. Physical Chemistry Chemical Physics, 2013, 15, 3772.	1.3	30
20	New insight into the electronic structure of iron(IV)â€oxo porphyrin compound I. A quantum chemical topological analysis. Journal of Computational Chemistry, 2013, 34, 780-789.	1.5	3
21	Role of Solvent on Nonenzymatic Peptide Bond Formation Mechanisms and Kinetic Isotope Effects. Journal of the American Chemical Society, 2013, 135, 8708-8719.	6.6	23
22	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
23	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
24	Do zwitterionic species exist in the non-enzymatic peptide bond formation?. Chemical Communications, 2012, 48, 11253.	2.2	8
25	Understanding the different activities of highly promiscuous MbtI by computational methods. Physical Chemistry Chemical Physics, 2012, 14, 3482.	1.3	16
26	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
27	Computational Analysis of Human OGA Structure in Complex with PUGNAc and NAG-Thiazoline Derivatives. Journal of Chemical Information and Modeling, 2012, 52, 2775-2783.	2.5	19
28	Theoretical studies of HIV-1 reverse transcriptase inhibition. Physical Chemistry Chemical Physics, 2012, 14, 12614.	1.3	24
29	A Collective Coordinate to Obtain Free Energy Profiles for Complex Reactions in Condensed Phases. Journal of Chemical Theory and Computation, 2012, 8, 1795-1801.	2.3	20
30	Hybrid Schemes Based on Quantum Mechanics/Molecular Mechanics Simulations. Advances in Protein Chemistry and Structural Biology, 2011, 85, 81-142.	1.0	19
31	Enzyme Molecular Mechanism as a Starting Point to Design New Inhibitors: A Theoretical Study of O-GlcNAcase. Journal of Physical Chemistry B, 2011, 115, 6764-6775.	1.2	24
32	A QM/MM study of the complexes formed by aluminum and iron with serum transferrin at neutral and acidic pH. Journal of Inorganic Biochemistry, 2011, 105, 1446-1456.	1.5	30
33	Temperature Dependence of the Kinetic Isotope Effects in Thymidylate Synthase. A Theoretical Study. Journal of the American Chemical Society, 2011, 133, 6692-6702.	6.6	60
34	Molecular mechanism of chorismate mutase activity of promiscuos MbtI. Theoretical Chemistry Accounts, 2011, 128, 601-607.	0.5	8
35	Theoretical QM/MM studies of enzymatic pericyclic reactions. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 115-131.	2.2	8
36	Application of Groteâ˜Hynes Theory to the Reaction Catalyzed by Thymidylate Synthase. Journal of Physical Chemistry B, 2010, 114, 13593-13600.	1.2	17

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37	Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation of Wild-Type and Seven Mutants of CpNagJ in Complex with PUGNAc. Journal of Physical Chemistry B, 2010, 114, 7029-7036.	1.2	16
38	Theoretical study of the temperature dependence of dynamic effects in thymidylate synthase. Physical Chemistry Chemical Physics, 2010, 12, 11657.	1.3	15
39	Computational Modeling of Biological Systems: The LDH Story. Challenges and Advances in Computational Chemistry and Physics, 2010, , 355-374.	0.6	0
40	Multipoint molecular recognition within a calix[6]arene funnel complex. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 10449-10454.	3.3	43
41	QM/MM Study of Thymidylate Synthase: Enzymatic Motions and the Temperature Dependence of the Rate Limiting Step. Journal of Physical Chemistry A, 2009, 113, 2176-2182.	1.1	31
42	Mechanism and Plasticity of Isochorismate Pyruvate Lyase: A Computational Study. Journal of the American Chemical Society, 2009, 131, 16156-16161.	6.6	28
43	Theoretical Modeling of the Reaction Mechanism of Phosphate Monoester Hydrolysis in Alkaline Phosphatase. Journal of Physical Chemistry B, 2009, 113, 7816-7824.	1.2	41
44	Toward Understanding the Photochemistry of Photoactive Yellow Protein: A CASPT2/CASSCF and Quantum Theory of Atoms in Molecules Combined Study of a Model Chromophore in Vacuo. Journal of Chemical Theory and Computation, 2009, 5, 3032-3038.	2.3	30
45	Theoretical Study of Catalytic Efficiency of a Dielsâ€“Alderase Catalytic Antibody: An Indirect Effect Produced During the Maturation Process. Chemistry - A European Journal, 2008, 14, 596-602.	1.7	9
46	A Quantum Mechanic/Molecular Mechanic Study of the Wild-Type and N155S Mutant HIV-1 Integrase Complexed with Diketo Acid. Biophysical Journal, 2008, 94, 2443-2451.	0.2	23
47	Computational design of biological catalysts. Chemical Society Reviews, 2008, 37, 2634.	18.7	41
48	A Theoretical Study of the Catalytic Mechanism of Formate Dehydrogenase. Journal of Physical Chemistry B, 2008, 112, 10012-10022.	1.2	46
49	A Quantum Mechanics/Molecular Mechanics Study of the Proteinâ^'Ligand Interaction of Two Potent Inhibitors of Human O-GlcNAcase: PUGNAc and NAG-Thiazoline. Journal of Physical Chemistry B, 2008, 112, 14260-14266.	1.2	27
50	Origin of the Absorption Maxima of the Photoactive Yellow Protein Resolved via Ab Initio Multiconfigurational Methods. Journal of Physical Chemistry B, 2008, 112, 7153-7156.	1.2	31
51	Predicting an Improvement of Secondary Catalytic Activity of Promiscuos Isochorismate Pyruvate Lyase by Computational Design. Journal of the American Chemical Society, 2008, 130, 2894-2895.	6.6	25
52	The effect of MM polarization on the QM/MM transition state stabilization: application to chorismate mutase. Molecular Physics, 2008, 106, 1511-1515.	0.8	13
53	Analysis of the Decarboxylation Step in Mammalian Histidine Decarboxylase. Journal of Biological Chemistry, 2008, 283, 12393-12401.	1.6	24
54	Long Distance Electron-Transfer Mechanism in Peptidylglycine Î±-Hydroxylating Monooxygenase:â€‰ A Perfect Fitting for a Water Bridge. Journal of the American Chemical Society, 2007, 129, 11700-11707.	6.6	33

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55	A Quantum Mechanics/Molecular Mechanics Study of the Catalytic Mechanism of the Thymidylate Synthaseâ€. Biochemistry, 2007, 46, 3704-3713.	1.2	35
56	A Quantum Mechanics/Molecular Mechanics Study of the Proteinâ€“Ligand Interaction for Inhibitors of HIV-1 Integrase. Chemistry - A European Journal, 2007, 13, 7715-7724.	1.7	38
57	Computer-Aided Rational Design of Catalytic Antibodies: The 1F7 Case. Angewandte Chemie - International Edition, 2007, 46, 286-290.	7.2	24
58	Calculation of binding energy using BLYP/MM for the HIV-1 integrase complexed with the S-1360 and two analogues. Bioorganic and Medicinal Chemistry, 2007, 15, 3818-3824.	1.4	17
59	Improving the QM/MM Description of Chemical Processes:â€‰ A Dual Level Strategy To Explore the Potential Energy Surface in Very Large Systems. [J. Chem. Theory Comput. 1, 1008â^'1016 (2005)]. Journal of Chemical Theory and Computation, 2006, 2, 216-216.	2.3	9
60	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
61	Stereoselectivity Behavior of the AZ28 Antibody Catalyzed Oxy-Cope Rearrangementâ€. Journal of Physical Chemistry A, 2006, 110, 726-730.	1.1	3
62	A Theoretical Analysis of Rate Constants and Kinetic Isotope Effects Corresponding to Different Reactant Valleys in Lactate Dehydrogenase. Journal of the American Chemical Society, 2006, 128, 16851-16863.	6.6	52
63	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. Angewandte Chemie - International Edition, 2005, 44, 904-909.	7.2	9
64	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. Angewandte Chemie, 2005, 117, 926-931.	1.6	3
65	Computing Kinetic Isotope Effects for Chorismate Mutase with High Accuracy. A New DFT/MM Strategy. Journal of Physical Chemistry B, 2005, 109, 3707-3710.	1.2	29
66	Improving the QM/MM Description of Chemical Processes:Â A Dual Level Strategy To Explore the Potential Energy Surface in Very Large Systems. Journal of Chemical Theory and Computation, 2005, 1, 1008-1016.	2.3	120
67	Electrostatic effects in enzyme catalysis: a quantum mechanics/molecular mechanics study of the nucleophilic substitution reaction in haloalkane dehalogenase. Theoretical Chemistry Accounts, 2004, 112, 327.	0.5	11
68	Vibrational analysis of the chorismate rearrangement: relaxed force constants, isotope effects and activation entropies calculated for reaction in vacuum, water and the active site of chorismate mutase. Journal of Physical Organic Chemistry, 2004, 17, 592-601.	0.9	28
69	Hybrid QM/MM Potentials of Mean Force with Interpolated Corrections. Journal of Physical Chemistry B, 2004, 108, 8427-8433.	1.2	95
70	A Comparative Study of Claisen and Cope Rearrangements Catalyzed by Chorismate Mutase. An Insight into Enzymatic Efficiency:Â Transition State Stabilization or Substrate Preorganization?. Journal of the American Chemical Society, 2004, 126, 311-319.	6.6	45
71	Theoretical insights in enzyme catalysis. Chemical Society Reviews, 2004, 33, 98-107.	18.7	150
72	Preorganization and Reorganization as Related Factors in Enzyme Catalysis: The Chorismate Mutase Case. Chemistry - A European Journal, 2003, 9, 984-991.	1.7	57

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73	Conformational equilibrium of chorismate. A QM/MM theoretical study combining statistical simulations and geometry optimisations in gas phase and in aqueous solution. Computational and Theoretical Chemistry, 2003, 632, 197-206.	1.5	13
74	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
75	Catalytic Mechanism of Dihydrofolate Reductase Enzyme. A Combined Quantum-Mechanical/Molecular-Mechanical Characterization of the N5 Protonation Step. Journal of Physical Chemistry B, 2003, 107, 14036-14041.	1.2	24
76	QM/MM calculations of kinetic isotope effects in the chorismate mutase active site. Organic and Biomolecular Chemistry, 2003, 1, 483-487.	1.5	28
77	An AM1 theoretical study on the effect of Zn2+ Lewis acid catalysis on the mechanism of the cycloaddition between 3-phenyl-1-(2-pyridyl)-2-propen-1-one and cyclopentadiene. Tetrahedron, 2002, 58, 2695-2700.	1.0	15
78	A Hybrid Potential Reaction Path and Free Energy Study of the Chorismate Mutase Reaction. Journal of the American Chemical Society, 2001, 123, 1709-1712.	6.6	92
79	Transition structure selectivity in enzyme catalysis: a QM/MM study of chorismate mutase. Theoretical Chemistry Accounts, 2001, 105, 207-212.	0.5	44
80	A QM/MM Study of the Conformational Equilibria in the Chorismate Mutase Active Site. The Role of the Enzymatic Deformation Energy Contribution. Journal of Physical Chemistry B, 2000, 104, 11308-11315.	1.2	54