

# Iñaki Tuñán

## List of Publications by Year in descending order

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197  
papers

6,229  
citations

76031

42  
h-index

111975

67  
g-index

210  
all docs

210  
docs citations

210  
times ranked

5632  
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. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4005-4013.	2.3	9
2	Spatial and Temporal Resolution of the Oxygen-Independent Photoinduced DNA Interstrand Cross-Linking by a Nitroimidazole Derivative. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3239-3252.	2.5	6
3	How a Second Mg <sup>2+</sup> Ion Affects the Phosphoryl-Transfer Mechanism in a Protein Kinase: A Computational Study. <i>ACS Catalysis</i> , 2021, 11, 169-183.	5.5	7
4	Computational simulations on the binding and reactivity of a nitrile inhibitor of the SARS-CoV-2 main protease. <i>Chemical Communications</i> , 2021, 57, 9096-9099.	2.2	32
5	Multiscale Simulations of SARS-CoV-2 3CL Protease Inhibition with Aldehyde Derivatives. Role of Protein and Inhibitor Conformational Changes in the Reaction Mechanism. <i>ACS Catalysis</i> , 2021, 11, 4157-4168.	5.5	40
6	Mechanistic study of the biosynthesis of R-phenylcarbinol by acetohydroxyacid synthase enzyme using hybrid quantum mechanics/molecular mechanics simulations. <i>Archives of Biochemistry and Biophysics</i> , 2021, 701, 108807.	1.4	1
7	Targeting the JAK/STAT Pathway: A Combined Ligand- and Target-Based Approach. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3091-3108.	2.5	8
8	Exploration of the Activation Mechanism of the Epigenetic Regulator MLL3: A QM/MM Study. <i>Biomolecules</i> , 2021, 11, 1051.	1.8	3
9	Inhibition Mechanism of SARS-CoV-2 Main Protease with Ketone-Based Inhibitors Unveiled by Multiscale Simulations: Insights for Improved Designs**. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 25933-25941.	7.2	24
10	A microscopic description of SARS-CoV-2 main protease inhibition with Michael acceptors. Strategies for improving inhibitor design. <i>Chemical Science</i> , 2021, 12, 3489-3496.	3.7	40
11	Computational Insights Into Enzyme Catalysis. , 2020, , 560-577.		0
12	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.	5.5	9
13	Are Heme-Dependent Enzymes Always Using a Redox Mechanism? A Theoretical Study of the Kemp Elimination Catalyzed by a Promiscuous Aldoxime Dehydratase. <i>ACS Catalysis</i> , 2020, 10, 11110-11119.	5.5	7
14	Seeking the Source of Catalytic Efficiency of Lindane Dehydrochlorinase, LinA. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10353-10364.	1.2	1
15	On the Nature of the Enzyme-Substrate Complex and the Reaction Mechanism in Human Arginase I. A Combined Molecular Dynamics and QM/MM Study. <i>ACS Catalysis</i> , 2020, 10, 8321-8333.	5.5	9
16	Unraveling the SARS-CoV-2 Main Protease Mechanism Using Multiscale Methods. <i>ACS Catalysis</i> , 2020, 10, 12544-12554.	5.5	107
17	Hypoxia-Selective Dissociation Mechanism of a Nitroimidazole Nucleoside in a DNA Environment. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6750-6754.	2.1	19
18	The transition state and cognate concepts. <i>Advances in Physical Organic Chemistry</i> , 2019, 53, 29-68.	0.5	8

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19	Mechanistic insights into the phosphoryl transfer reaction in cyclin-dependent kinase 2: A QM/MM study. <i>PLoS ONE</i> , 2019, 14, e0215793.	1.1	8
20	Loss of Hyperconjugative Effects Drives Hydride Transfer during Dihydrofolate Reductase Catalysis. <i>ACS Catalysis</i> , 2019, 9, 10343-10349.	5.5	1
21	Studying the phosphoryl transfer mechanism of the <i>E. coli</i> phosphofructokinase-2: from X-ray structure to quantum mechanics/molecular mechanics simulations. <i>Chemical Science</i> , 2019, 10, 2882-2892.	3.7	15
22	Why Are Some Enzymes Dimers? Flexibility and Catalysis in <i>Thermotoga maritima</i> Dihydrofolate Reductase. <i>ACS Catalysis</i> , 2019, 9, 5902-5911.	5.5	12
23	Heavy Enzymes and the Rational Redesign of Protein Catalysts. <i>ChemBioChem</i> , 2019, 20, 2807-2812.	1.3	5
24	A first peek into sub-picosecond dynamics of spin energy levels in magnetic biomolecules. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10908-10913.	1.3	7
25	Modeling caspase-1 inhibition: Implications for catalytic mechanism and drug design. <i>European Journal of Medicinal Chemistry</i> , 2019, 169, 159-167.	2.6	8
26	Translocation of Enzymes into a Mesoporous MOF for Enhanced Catalytic Activity Under Extreme Conditions. <i>Chemical Science</i> , 2019, 10, 4082-4088.	3.7	47
27	A molecular dynamics study on the role of the protonation state in the biosynthesis of R-PAC by AHAS. <i>Chemical Physics Letters</i> , 2019, 716, 247-251.	1.2	4
28	Insights on the Origin of Catalysis on Glycine <i>N</i> -Methyltransferase from Computational Modeling. <i>Journal of the American Chemical Society</i> , 2018, 140, 4327-4334.	6.6	48
29	Isotope Substitution of Promiscuous Alcohol Dehydrogenase Reveals the Origin of Substrate Preference in the Transition State. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 3128-3131.	7.2	10
30	Origin of Enzymatic Kinetic Isotope Effects in Human Purine Nucleoside Phosphorylase. <i>ACS Catalysis</i> , 2018, 8, 815-827.	5.5	5
31	Dynamics of the excited-state hydrogen transfer in a (dG) $\hat{A}$ ·(dC) homopolymer: intrinsic photostability of DNA. <i>Chemical Science</i> , 2018, 9, 7902-7911.	3.7	29
32	Catalytic Reaction Mechanism in Native and Mutant Catechol- <i>O</i> -methyltransferase from the Adaptive String Method and Mean Reaction Force Analysis. <i>Journal of Physical Chemistry B</i> , 2018, 122, 8861-8871.	1.2	8
33	Isotope Substitution of Promiscuous Alcohol Dehydrogenase Reveals the Origin of Substrate Preference in the Transition State. <i>Angewandte Chemie</i> , 2018, 130, 3182-3185.	1.6	2
34	Reaction coordinates and transition states in enzymatic catalysis. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1329.	6.2	27
35	Molecular Mechanism of Inhibition of DNA Methylation by Zebularine. <i>ACS Catalysis</i> , 2017, 7, 1728-1732.	5.5	7
36	Free energy profiles for two ubiquitous damaging agents: methylation and hydroxylation of guanine in B-DNA. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 14695-14701.	1.3	3

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37	A DFT study on the chiral synthesis of R-phenylacetyl carbinol within the quantum chemical cluster approach. <i>Chemical Physics Letters</i> , 2017, 677, 30-34.	1.2	5
38	Revealing the Origin of the Efficiency of the De Novo Designed Kemp Eliminase HGâ€³.17 by Comparison with the Former Developed HGâ€³. <i>Chemistry - A European Journal</i> , 2017, 23, 7582-7589.	1.7	16
39	Convergence of Theory and Experiment on the Role of Preorganization, Quantum Tunneling, and Enzyme Motions into Flavoenzyme-Catalyzed Hydride Transfer. <i>ACS Catalysis</i> , 2017, 7, 3190-3198.	5.5	31
40	Regioselectivity of the OH Radical Addition to Uracil in Nucleic Acids. A Theoretical Approach Based on QM/MM Simulations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5089-5096.	2.3	13
41	Adaptive Finite Temperature String Method in Collective Variables. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9764-9772.	1.1	40
42	Quantifying the limits of transition state theory in enzymatic catalysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 12390-12395.	3.3	22
43	Molecular mechanism of the site-specific self-cleavage of the RNA phosphodiester backbone by a twister ribozyme. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	6
44	Insights into the inhibited form of the redox-sensitive SufE-like sulfur acceptor CsdE. <i>PLoS ONE</i> , 2017, 12, e0186286.	1.1	0
45	Thermal Isomerization Mechanism in Dronpa and Its Mutants. <i>Journal of Physical Chemistry B</i> , 2016, 120, 12820-12825.	1.2	9
46	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.	5.5	30
47	Mechanism of Sulfur Transfer Across Proteinâ€“Protein Interfaces: The Cysteine Desulfurase Model System. <i>ACS Catalysis</i> , 2016, 6, 3975-3984.	5.5	12
48	Singlet Oxygen Attack on Guanine: Reactivity and Structural Signature within the Bâ€“DNA Helix. <i>Chemistry - A European Journal</i> , 2016, 22, 12358-12362.	1.7	34
49	DFT Study on the Interaction of Tris(benzene-1,2-dithiolato)molybdenum Complex with Water. A Hydrolysis Mechanism Involving a Feasible Seven-Coordinate Aquomolybdenum Intermediate. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9636-9646.	1.1	5
50	Minimization of dynamic effects in the evolution of dihydrofolate reductase. <i>Chemical Science</i> , 2016, 7, 3248-3255.	3.7	25
51	Chapter 3. A Transition State Theory Perspective for Enzymatic Reactions: Fundamentals and Applications. <i>RSC Theoretical and Computational Chemistry Series</i> , 2016, , 54-88.	0.7	0
52	Chemical Ligation and Isotope Labeling to Locate Dynamic Effects during Catalysis by Dihydrofolate Reductase. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 9016-9020.	7.2	35
53	Transition state ensemble optimization for reactions of arbitrary complexity. <i>Journal of Chemical Physics</i> , 2015, 143, 134111.	1.2	5
54	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.	1.2	6

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55	Protein Conformational Landscapes and Catalysis. Influence of Active Site Conformations in the Reaction Catalyzed by L-Lactate Dehydrogenase. <i>ACS Catalysis</i> , 2015, 5, 1172-1185.	5.5	48
56	Are there dynamical effects in enzyme catalysis? Some thoughts concerning the enzymatic chemical step. <i>Archives of Biochemistry and Biophysics</i> , 2015, 582, 42-55.	1.4	36
57	Computational strategies for the design of new enzymatic functions. <i>Archives of Biochemistry and Biophysics</i> , 2015, 582, 68-79.	1.4	49
58	Protein Flexibility and Preorganization in the Design of Enzymes. The Kemp Elimination Catalyzed by HG3.17. <i>ACS Catalysis</i> , 2015, 5, 2587-2595.	5.5	28
59	Peptide Bond Formation Mechanism Catalyzed by Ribosome. <i>Journal of the American Chemical Society</i> , 2015, 137, 12024-12034.	6.6	34
60	Dehydrochlorination of Hexachlorocyclohexanes Catalyzed by the LinA Dehydrohalogenase. A QM/MM Study. <i>Journal of Physical Chemistry B</i> , 2015, 119, 15100-15109.	1.2	19
61	Linking Electrostatic Effects and Protein Motions in Enzymatic Catalysis. A Theoretical Analysis of Catechol <i>o</i> -Methyltransferase. <i>Journal of Physical Chemistry B</i> , 2015, 119, 873-882.	1.2	14
62	Exploring Chemical Reactivity in Enzyme Catalyzed Processes Using QM/MM Methods: An Application to Dihydrofolate Reductase. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 383-413.	0.6	1
63	Exploring chemical reactivity of complex systems with path-based coordinates: Role of the distance metric. <i>Journal of Computational Chemistry</i> , 2014, 35, 1672-1681.	1.5	15
64	Protein Isotope Effects in Dihydrofolate Reductase From <i>Geobacillus stearothermophilus</i> Show Entropic-Enthalpic Compensatory Effects on the Rate Constant. <i>Journal of the American Chemical Society</i> , 2014, 136, 17317-17323.	6.6	34
65	Dynamics and Reactivity in <i>Thermus aquaticus</i> N6-Adenine Methyltransferase. <i>Journal of the American Chemical Society</i> , 2014, 136, 16227-16239.	6.6	22
66	Predicting enzymatic reactivity: from theory to design. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 407-421.	6.2	32
67	The Catalytic Mechanism of Carboxylesterases: A Computational Study. <i>Biochemistry</i> , 2014, 53, 5820-5829.	1.2	53
68	Heavy enzymes—experimental and computational insights in enzyme dynamics. <i>Current Opinion in Chemical Biology</i> , 2014, 21, 11-18.	2.8	39
69	The catalytic mechanism of glyceraldehyde 3-phosphate dehydrogenase from <i>Trypanosoma cruzi</i> elucidated via the QM/MM approach. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3772.	1.3	30
70	Toward an Automatic Determination of Enzymatic Reaction Mechanisms and Their Activation Free Energies. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3740-3749.	2.3	37
71	Role of Solvent on Nonenzymatic Peptide Bond Formation Mechanisms and Kinetic Isotope Effects. <i>Journal of the American Chemical Society</i> , 2013, 135, 8708-8719.	6.6	23
72	Studying the role of protein dynamics in an SN2 enzyme reaction using free-energy surfaces and solvent coordinates. <i>Nature Chemistry</i> , 2013, 5, 566-571.	6.6	49

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73	Increased Dynamic Effects in a Catalytically Compromised Variant of <i>Escherichia coli</i> Dihydrofolate Reductase. <i>Journal of the American Chemical Society</i> , 2013, 135, 18689-18696.	6.6	56
74	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.	3.3	119
75	Modeling methods for studying post-translational and transcriptional modifying enzymes. <i>Current Opinion in Chemical Biology</i> , 2012, 16, 465-471.	2.8	5
76	Do zwitterionic species exist in the non-enzymatic peptide bond formation?. <i>Chemical Communications</i> , 2012, 48, 11253.	2.2	8
77	Understanding the different activities of highly promiscuous Mbtl by computational methods. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 3482.	1.3	16
78	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. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1532-1535.	2.3	10
79	A Collective Coordinate to Obtain Free Energy Profiles for Complex Reactions in Condensed Phases. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1795-1801.	2.3	20
80	Enzyme dynamics and catalysis in the mechanism of DNA polymerase. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	16
81	Substrate promiscuity in DNA methyltransferase M.Pvull. A mechanistic insight. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 5395.	1.5	8
82	Computational study on hydrolysis of cefotaxime in gas phase and in aqueous solution. <i>Journal of Computational Chemistry</i> , 2012, 33, 1948-1959.	1.5	6
83	Hydrolysis of Phosphotriesters: A Theoretical Analysis of the Enzymatic and Solution Mechanisms. <i>Chemistry - A European Journal</i> , 2012, 18, 9612-9621.	1.7	26
84	Reversibility and Diffusion in Mandelythiamin Decarboxylation. Searching Dynamical Effects in Decarboxylation Reactions. <i>Journal of the American Chemical Society</i> , 2012, 134, 10509-10514.	6.6	8
85	Tetraethylorthosilicate as molecular precursor to the formation of amorphous silica networks. A DFT-SCRF study of the base catalyzed hydrolysis. <i>Journal of Molecular Modeling</i> , 2012, 18, 3301-3310.	0.8	12
86	Hybrid Schemes Based on Quantum Mechanics/Molecular Mechanics Simulations. <i>Advances in Protein Chemistry and Structural Biology</i> , 2011, 85, 81-142.	1.0	19
87	Enzyme Molecular Mechanism as a Starting Point to Design New Inhibitors: A Theoretical Study of <i>O</i> -GlcNAcase. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6764-6775.	1.2	24
88	Promiscuity in Alkaline Phosphatase Superfamily. Unraveling Evolution through Molecular Simulations. <i>Journal of the American Chemical Society</i> , 2011, 133, 12050-12062.	6.6	61
89	Molecular mechanism of chorismate mutase activity of promiscuous Mbtl. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 601-607.	0.5	8
90	A Simple Model for Barrier Frequencies for Enzymatic Reactions. <i>ChemPhysChem</i> , 2011, 12, 184-190.	1.0	2

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91	Does glycosyl transfer involve an oxacarbenium intermediate? Computational simulation of the lifetime of the methoxymethyl cation in water. <i>Pure and Applied Chemistry</i> , 2011, 83, 1507-1514.	0.9	9
92	Theoretical QM/MM studies of enzymatic pericyclic reactions. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2010, 2, 115-131.	2.2	8
93	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.	1.7	25
94	<i>digitalis purpurea</i> P512R2, encoding steroid 5 $\beta$ -reductase, is a novel defense-related gene involved in cardenolide biosynthesis. <i>New Phytologist</i> , 2010, 185, 687-700.	3.5	57
95	Application of Grote's Hynes Theory to the Reaction Catalyzed by Thymidylate Synthase. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13593-13600.	1.2	17
96	Computational Simulation of the Lifetime of the Methoxymethyl Cation in Water. A Simple Model for a Glycosyl Cation: When Is an Intermediate an Intermediate?. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5769-5774.	1.2	11
97	Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation of Wild-Type and Seven Mutants of <i>CpNagI</i> in Complex with PUGNAc. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7029-7036.	1.2	16
98	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
99	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
100	Theoretical study of the temperature dependence of dynamic effects in thymidylate synthase. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11657.	1.3	15
101	Computational Modeling of Biological Systems: The LDH Story. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2010, , 355-374.	0.6	0
102	A QM/MM study of the reaction mechanism for the 3'-processing step catalyzed by HIV-1 integrase. <i>Computational and Theoretical Chemistry</i> , 2009, 898, 115-120.	1.5	8
103	Theoretical Modeling on the Reaction Mechanism of p-Nitrophenylmethylphosphate Alkaline Hydrolysis and its Kinetic Isotope Effects. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 439-442.	2.3	16
104	Mechanism and Plasticity of Isochorismate Pyruvate Lyase: A Computational Study. <i>Journal of the American Chemical Society</i> , 2009, 131, 16156-16161.	6.6	28
105	Theoretical Modeling of the Reaction Mechanism of Phosphate Monoester Hydrolysis in Alkaline Phosphatase. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7816-7824.	1.2	41
106	Critical Role of Substrate Conformational Change in the Proton Transfer Process Catalyzed by 4-Oxalocrotonate Tautomerase. <i>Journal of the American Chemical Society</i> , 2009, 131, 2687-2698.	6.6	18
107	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
108	Theoretical Study of Catalytic Efficiency of a Diels-Alderase Catalytic Antibody: An Indirect Effect Produced During the Maturation Process. <i>Chemistry - A European Journal</i> , 2008, 14, 596-602.	1.7	9

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109	A Quantum Mechanic/Molecular Mechanic Study of the Wild-Type and N155S Mutant HIV-1 Integrase Complexed with Diketo Acid. <i>Biophysical Journal</i> , 2008, 94, 2443-2451.	0.2	23
110	Theoretical site-directed mutagenesis: Asp168Ala mutant of lactate dehydrogenase. <i>Journal of the Royal Society Interface</i> , 2008, 5, 217-224.	1.5	3
111	Computational design of biological catalysts. <i>Chemical Society Reviews</i> , 2008, 37, 2634.	18.7	41
112	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
113	Using Groteâ~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
114	A Quantum Mechanics/Molecular Mechanics Study of the Proteinâ~Ligand Interaction of Two Potent Inhibitors of Human O-GlcNAcase: PUGNAc and NAG-Thiazoline. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14260-14266.	1.2	27
115	Predicting an Improvement of Secondary Catalytic Activity of Promiscuous Isochorismate Pyruvate Lyase by Computational Design. <i>Journal of the American Chemical Society</i> , 2008, 130, 2894-2895.	6.6	25
116	Analysis of the Decarboxylation Step in Mammalian Histidine Decarboxylase. <i>Journal of Biological Chemistry</i> , 2008, 283, 12393-12401.	1.6	24
117	Enzymatic Effects on Reactant and Transition States. The Case of Chalcone Isomerase. <i>Journal of the American Chemical Society</i> , 2007, 129, 9117-9124.	6.6	16
118	A Computational Study of the Protein-Ligand Interactions in CDK2 Inhibitors: Using Quantum Mechanics/Molecular Mechanics Interaction Energy as a Predictor of the Biological Activity. <i>Biophysical Journal</i> , 2007, 92, 430-439.	0.2	49
119	A Quantum Mechanics/Molecular Mechanics Study of the Proteinâ€“Ligand Interaction for Inhibitors of HIV-1 Integrase. <i>Chemistry - A European Journal</i> , 2007, 13, 7715-7724.	1.7	38
120	Computer-Aided Rational Design of Catalytic Antibodies: The 1F7 Case. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 286-290.	7.2	24
121	Calculation of binding energy using BLYP/MM for the HIV-1 integrase complexed with the S-1360 and two analogues. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 3818-3824.	1.4	17
122	Improving the QM/MM Description of Chemical Processes:â€“ A Dual Level Strategy To Explore the Potential Energy Surface in Very Large Systems. [ <i>J. Chem. Theory Comput.</i> 1, 1008â“1016 (2005)]. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 216-216.	2.3	9
123	Hybrid Quantum Mechanics/Molecular Mechanics Simulations with Two-Dimensional Interpolated Corrections:â€“ Application to Enzymatic Processes. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17663-17670.	1.2	57
124	Coupling between Protein and Reaction Dynamics in Enzymatic Processes:â€“ Application of Groteâ~Hynes Theory to CatecholO-Methyltransferase. <i>Journal of the American Chemical Society</i> , 2006, 128, 6186-6193.	6.6	57
125	Stereoselectivity Behavior of the AZ28 Antibody Catalyzed Oxy-Cope Rearrangementâ€. <i>Journal of Physical Chemistry A</i> , 2006, 110, 726-730.	1.1	3
126	Activation Free Energy of CatecholO-Methyltransferase. Corrections to the Potential of Mean Forceâ€. <i>Journal of Physical Chemistry A</i> , 2006, 110, 503-509.	1.1	32



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127	A Theoretical Analysis of Rate Constants and Kinetic Isotope Effects Corresponding to Different Reactant Valleys in Lactate Dehydrogenase. <i>Journal of the American Chemical Society</i> , 2006, 128, 16851-16863.	6.6	52
128	Comparative Computational Analysis of Different Active Site Conformations and Substrates in a Chalcone Isomerase Catalyzed Reaction. <i>Journal of Physical Chemistry B</i> , 2006, 110, 20686-20692.	1.2	15
129	Catalysis in Glycine N-Methyltransferase: Testing the Electrostatic Stabilization and Compression Hypothesis. <i>Biochemistry</i> , 2006, 45, 14917-14925.	1.2	28
130	FT-Raman and QM/MM study of the interaction between histamine and DNA. <i>Chemical Physics</i> , 2006, 324, 579-590.	0.9	26
131	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 904-909.	7.2	9
132	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. <i>Angewandte Chemie</i> , 2005, 117, 926-931.	1.6	3
133	The Mechanism of Formamide Hydrolysis in Water from Ab Initio Calculations and Simulations. <i>Chemistry - A European Journal</i> , 2005, 11, 6743-6753.	1.7	90
134	Dependence of enzyme reaction mechanism on protonation state of titratable residues and QM level description: lactate dehydrogenase. <i>Chemical Communications</i> , 2005, , 5873.	2.2	17
135	On the Nature of the Transition State in Catechol O-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
136	Dynamic and Electrostatic Effects in Enzymatic Processes. An Analysis of the Nucleophilic Substitution Reaction in Haloalkane Dehalogenase. <i>Journal of the American Chemical Society</i> , 2005, 127, 1946-1957.	6.6	42
137	Computing Kinetic Isotope Effects for Chorismate Mutase with High Accuracy. A New DFT/MM Strategy. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3707-3710.	1.2	29
138	Improving the QM/MM Description of Chemical Processes: A Dual Level Strategy To Explore the Potential Energy Surface in Very Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1008-1016.	2.3	120
139	A QM/MM Exploration of the Potential Energy Surface of Pyruvate to Lactate Transformation Catalyzed by LDH. Improving the Accuracy of Semiempirical Descriptions. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 750-761.	2.3	22
140	Electrostatic effects in enzyme catalysis: a quantum mechanics/molecular mechanics study of the nucleophilic substitution reaction in haloalkane dehalogenase. <i>Theoretical Chemistry Accounts</i> , 2004, 112, 327.	0.5	11
141	Theoretical Insights in Enzyme Catalysis. <i>ChemInform</i> , 2004, 35, no.	0.1	0
142	Amino acid chemistry in solution: structural properties and vibrational dynamics of serine using density functional theory and a continuum solvent model. <i>Chemical Physics</i> , 2004, 303, 85-96.	0.9	33
143	Hybrid QM/MM Potentials of Mean Force with Interpolated Corrections. <i>Journal of Physical Chemistry B</i> , 2004, 108, 8427-8433.	1.2	95
144	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

#	ARTICLE	IF	CITATIONS
145	A Comparative Study of Claisen and Cope Rearrangements Catalyzed by Chorismate Mutase. An Insight into Enzymatic Efficiency:Ä Transition State Stabilization or Substrate Preorganization?. <i>Journal of the American Chemical Society</i> , 2004, 126, 311-319.	6.6	45
146	Theoretical insights in enzyme catalysis. <i>Chemical Society Reviews</i> , 2004, 33, 98-107.	18.7	150
147	Fundamental Principles Governing Solvent Use: Solvent Effects on Chemical Systems. <i>ChemInform</i> , 2003, 34, no.	0.1	0
148	Preorganization and Reorganization as Related Factors in Enzyme Catalysis: The Chorismate Mutase Case. <i>Chemistry - A European Journal</i> , 2003, 9, 984-991.	1.7	57
149	A theoretical study of solvent effects on the conformational equilibria of neutral glycine in aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2003, 623, 203-210.	1.5	24
150	Conformational equilibrium of chorismate. A QM/MM theoretical study combining statistical simulations and geometry optimisations in gas phase and in aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2003, 632, 197-206.	1.5	13
151	Theoretical Modeling of Enzyme Catalytic Power:Ä Analysis of äœCraticä€and Electrostatic Factors in CatecholO-Methyltransferase. <i>Journal of the American Chemical Society</i> , 2003, 125, 7726-7737.	6.6	79
152	Internal Rotation of 1,2-Dichloroethane in Haloalkane Dehalogenase. A Test Case for Analyzing Electrostatic Effects in Enzymes. <i>Journal of Physical Chemistry B</i> , 2003, 107, 6234-6238.	1.2	14
153	Structural and Vibrational Study of the Tautomerism of Histamine Free-Base in Solution. <i>Journal of the American Chemical Society</i> , 2003, 125, 2328-2340.	6.6	50
154	Catalytic Mechanism of Dihydrofolate Reductase Enzyme. A Combined Quantum-Mechanical/Molecular-Mechanical Characterization of the N5 Protonation Step. <i>Journal of Physical Chemistry B</i> , 2003, 107, 14036-14041.	1.2	24
155	QM/MM calculations of kinetic isotope effects in the chorismate mutase active site. <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 483-487.	1.5	28
156	Role of Protein Flexibility in Enzymatic Catalysis:ä€ Quantum Mechanicalä~Molecular Mechanical Study of the Deacylation Reaction in Class A Î²-Lactamases. <i>Journal of the American Chemical Society</i> , 2002, 124, 1809-1816.	6.6	31
157	A quantum mechanics-molecular mechanics study of dissociative electron transfer: The methylchloride radical anion in aqueous solution. <i>Journal of Chemical Physics</i> , 2002, 116, 6102-6110.	1.2	7
158	Water-Assisted Alkaline Hydrolysis of Monobactams: A Theoretical Study. <i>Chemistry - A European Journal</i> , 2002, 8, 859-867.	1.7	13
159	A Hybrid Potential Reaction Path and Free Energy Study of the Chorismate Mutase Reaction. <i>Journal of the American Chemical Society</i> , 2001, 123, 1709-1712.	6.6	92
160	Transition structure selectivity in enzyme catalysis: a QM/MM study of chorismate mutase. <i>Theoretical Chemistry Accounts</i> , 2001, 105, 207-212.	0.5	44
161	On the tautomerization process of glycine in aqueous solution. <i>Chemical Physics Letters</i> , 2000, 321, 433-437.	1.2	57
162	Intramolecular proton transfer of serine in aqueous solution. Mechanism and energetics. <i>Theoretical Chemistry Accounts</i> , 2000, 104, 89-95.	0.5	34

#	ARTICLE	IF	CITATIONS
163	A QM/MM Study of the Conformational Equilibria in the Chorismate Mutase Active Site. The Role of the Enzymatic Deformation Energy Contribution. <i>Journal of Physical Chemistry B</i> , 2000, 104, 11308-11315.	1.2	54
164	A quantum mechanics/molecular mechanics study of the acylation reaction of TEM1 Î²-lactamase and penicillanate. <i>Perkin Transactions II RSC</i> , 2000, , 761-767.	1.1	19
165	Molecular dynamics simulation in aqueous solution of N -methylazetidinone as a model of Î² -lactam antibiotics. <i>Theoretical Chemistry Accounts</i> , 1999, 101, 336-342.	0.5	8
166	Modeling Î³-lactam interactions in aqueous solution through combined quantum mechanics-molecular mechanics methods. <i>Journal of Computational Chemistry</i> , 1999, 20, 1401-1411.	1.5	16
167	Analysis of a concerted mechanism in Î²-lactam enzymatic hydrolysis. A quantum mechanics/molecular mechanics study. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 1351-1356.	0.9	8
168	The Solvent-Excluding Surface as a descriptor of ionic channels: Gramicidin-A. <i>Computational and Theoretical Chemistry</i> , 1998, 426, 331-338.	1.5	5
169	Neutral and Alkaline Hydrolyses of Model Î²-Lactam Antibiotics. An ab Initio Study of Water Catalysis. <i>Journal of the American Chemical Society</i> , 1998, 120, 2146-2155.	6.6	71
170	Aminoacid zwitterions in solution: Geometric, energetic, and vibrational analysis using density functional theory-continuum model calculations. <i>Journal of Chemical Physics</i> , 1998, 109, 592-603.	1.2	87
171	Intramolecular Proton Transfer of Glycine in Aqueous Solution Using Quantum MechanicsâMolecular Mechanics Simulations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 8673-8678.	1.1	68
172	Ab Initio Calculations on Neutral and Alkaline Hydrolyses of Î²-Lactam Antibiotics. A Theoretical Study Including Solvent Effects. <i>Journal of Physical Chemistry B</i> , 1997, 101, 3581-3588.	1.2	56
173	A Theoretical Study of the Favorskii Rearrangement. Calculation of Gas-Phase Reaction Paths and Solvation Effects on the Molecular Mechanism for the Transposition of the Î±-Chlorocyclobutanone. <i>Journal of the American Chemical Society</i> , 1997, 119, 1941-1947.	6.6	24
174	Rotational constants and dipole moments of interstellar polyynes: a comparative MP2 and density functional (BP86) study. <i>Chemical Physics</i> , 1996, 206, 57-61.	0.9	17
175	Correlation effects in proton transfer reactions in solution. <i>Computational and Theoretical Chemistry</i> , 1996, 371, 117-121.	1.5	6
176	Computation of hydration free energies using a parameterized continuum model: Study of equilibrium geometries and reactive processes in water solution. <i>Journal of Computational Chemistry</i> , 1996, 17, 148-155.	1.5	51
177	Can Hydrophobic Interactions Be Correctly Reproduced by the Continuum Models?. <i>The Journal of Physical Chemistry</i> , 1996, 100, 9955-9959.	2.9	32
178	Coupled density functional/molecular mechanics Monte Carlo simulations of ions in water. The bromide ion. <i>Chemical Physics Letters</i> , 1995, 241, 450-456.	1.2	51
179	A Hybrid Density Functional-Classical Molecular Dynamics Simulation of a Water Molecule in Liquid Water. <i>Journal of Molecular Modeling</i> , 1995, 1, 196-201.	0.8	51
180	Hydroxide Ion in Liquid Water: Structure, Energetics, and Proton Transfer Using a Mixed Discrete-Continuum ab Initio Model. <i>The Journal of Physical Chemistry</i> , 1995, 99, 3798-3805.	2.9	95

#	ARTICLE	IF	CITATIONS
181	Solvent Effects on the Thermodynamics and Kinetics of the Proton Transfer between Hydronium Ion and Ammonia. A Theoretical Study Using the Continuum and the Discrete Models. The Journal of Physical Chemistry, 1995, 99, 12525-12528.	2.9	12
182	GEPOL: An improved description of molecular surfaces. III. A new algorithm for the computation of a solvent-excluding surface. Journal of Computational Chemistry, 1994, 15, 1127-1138.	1.5	760
183	Transition structures of the Friedelâ€“Crafts reaction in solution. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1757-1761.	1.7	17
184	AB initio rotational constants of the nitriles derived from cyanodiacetylene (HC4CN). Astrophysical Journal, 1994, 437, 532.	1.6	10
185	Continuum-uniform approach calculations of the solubility of hydrocarbons in water. Chemical Physics Letters, 1993, 203, 289-294.	1.2	43
186	Ab initio rotational constants of interstellar species: Cyanoacetylene hydrogenated derivatives. International Journal of Quantum Chemistry, 1993, 46, 231-238.	1.0	2
187	Proton solvation in liquid water: an ab initio study using the continuum model. The Journal of Physical Chemistry, 1993, 97, 5547-5552.	2.9	59
188	Theoretical study of the inversion of the alcohol acidity scale in aqueous solution. Toward an interpretation of the acid-base behavior of organic compounds in solution. Journal of the American Chemical Society, 1993, 115, 2226-2230.	6.6	47
189	Proton transfer between water molecules: a theoretical study of solvent effects using the continuum and the discrete-continuum models. The Journal of Physical Chemistry, 1993, 97, 11087-11091.	2.9	25
190	AB Initio Rotational Constants of Isocyanopolynes. Astrophysical Journal, 1993, 415, L151.	1.6	10
191	Methylamines basicity calculations: in vacuo and in solution comparative analysis. The Journal of Physical Chemistry, 1992, 96, 9043-9048.	2.9	70
192	Molecular surface calculations on organic compounds. Computational and Theoretical Chemistry, 1992, 254, 369-377.	1.5	11
193	GEPOL: An improved description of molecular surfaces II. Computing the molecular area and volume. Journal of Computational Chemistry, 1991, 12, 1077-1088.	1.5	237
194	Theoretical rotational constants of MeCnN species. Chemical Physics Letters, 1990, 166, 54-56.	1.2	8
195	HCnN: The largest molecules in the interstellar medium. Journal of Chemical Education, 1990, 67, 905.	1.1	18
196	Theoretical Studies of the Self Cleavage Pistol Ribozyme Mechanism. Topics in Catalysis, 0, , 1.	1.3	3
197	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