

# Natalia Diaz

## List of Publications by Year in descending order

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72  
papers

1,622  
citations

279798

23  
h-index

330143

37  
g-index

73  
all docs

73  
docs citations

73  
times ranked

1941  
citing authors

#	ARTICLE	IF	CITATIONS
1	SARS-CoV-2 Main Protease: A Molecular Dynamics Study. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5815-5831.	5.4	112
2	Zinc Metallo- $\beta$ -Lactamase from <i>Bacteroides fragilis</i> : A Quantum Chemical Study on Model Systems of the Active Site. <i>Journal of the American Chemical Society</i> , 2000, 122, 4197-4208.	13.7	84
3	Ureases: Quantum Chemical Calculations on Cluster Models. <i>Journal of the American Chemical Society</i> , 2003, 125, 15324-15337.	13.7	82
4	Molecular Dynamics Study of the IIA Binding Site in Human Serum Albumin: Influence of the Protonation State of Lys195 and Lys199. <i>Journal of Medicinal Chemistry</i> , 2001, 44, 250-260.	6.4	74
5	Insights into the Phosphoryl-Transfer Mechanism of cAMP-Dependent Protein Kinase from Quantum Chemical Calculations and Molecular Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2004, 126, 529-542.	13.7	67
6	Molecular Dynamics Simulations of the Mononuclear Zinc- $\beta$ -lactamase from <i>Bacillus cereus</i> Complexed with Benzylpenicillin and a Quantum Chemical Study of the Reaction Mechanism. <i>Journal of the American Chemical Society</i> , 2001, 123, 9867-9879.	13.7	66
7	Insights into the Acylation Mechanism of Class A $\beta$ -Lactamases from Molecular Dynamics Simulations of the TEM-1 Enzyme Complexed with Benzylpenicillin. <i>Journal of the American Chemical Society</i> , 2003, 125, 672-684.	13.7	61
8	Entropy Calculations of Single Molecules by Combining the Rigid-Rotor and Harmonic-Oscillator Approximations with Conformational Entropy Estimations from Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2638-2653.	5.3	56
9	Molecular dynamics simulations of the dinuclear zinc- $\beta$ -lactamase from <i>Bacteroides fragilis</i> complexed with imipenem. <i>Journal of Computational Chemistry</i> , 2002, 23, 1587-1600.	3.3	52
10	Hydration of zinc ions: theoretical study of $[Zn(H_2O)_4](H_2O)_{82+}$ and $[Zn(H_2O)_6](H_2O)_{62+}$ . <i>Chemical Physics Letters</i> , 2000, 326, 288-292.	2.6	45
11	Acylation of Class A $\beta$ -lactamases by Penicillins: A Theoretical Examination of the Role of Serine 130 and the $\beta$ -lactam Carboxylate Group. <i>Journal of Physical Chemistry B</i> , 2001, 105, 11302-11313.	2.6	42
12	Direct methods for computing single-molecule entropies from molecular simulations. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2015, 5, 1-26.	14.6	39
13	Molecular Dynamics Simulations of Matrix Metalloproteinase 2: Role of the Structural Metal Ions. <i>Biochemistry</i> , 2007, 46, 8943-8952.	2.5	37
14	Thermochemical Fragment Energy Method for Biomolecules: Application to a Collagen Model Peptide. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1667-1679.	5.3	37
15	Monoligand Zn(II) Complexes: Ab Initio Benchmark Calculations and Comparison with Density Functional Theory Methodologies. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 243-256.	5.3	35
16	Peptide Hydrolysis Catalyzed by Matrix Metalloproteinase 2: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8412-8424.	2.6	32
17	CENCALC: A computational tool for conformational entropy calculations from molecular simulations. <i>Journal of Computational Chemistry</i> , 2013, 34, 2041-2054.	3.3	32
18	Progress towards water-soluble triazole-based selective MMP-2 inhibitors. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 6623.	2.8	31

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19	Theoretical Study of the Water-Assisted Aminolysis of $\beta$ -Lactams: Implications for the Reaction between Human Serum Albumin and Penicillins. <i>Journal of the American Chemical Society</i> , 2000, 122, 6710-6719.	13.7	29
20	Molecular Dynamics Simulations of the TEM-1 $\beta$ -Lactamase Complexed with Cephalothin. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 780-791.	6.4	29
21	Theoretical Studies on the Ring Opening of $\beta$ -lactams: Processes in Solution and in Enzymatic Media. <i>Current Organic Chemistry</i> , 2006, 10, 805-821.	1.6	28
22	An Integrated Computational and Experimental Approach to Gaining Selectivity for MMP-2 within the Gelatinase Subfamily. <i>ChemBioChem</i> , 2014, 15, 399-412.	2.6	24
23	A Theoretical Study of the Aminolysis Reaction of Lysine 199 of Human Serum Albumin with Benzylpenicillin: Consequences for Immunochemistry of Penicillins. <i>Journal of the American Chemical Society</i> , 2001, 123, 7574-7583.	13.7	23
24	A Computational Study of the Deacylation Mechanism of Human Butyrylcholinesterase. <i>Biochemistry</i> , 2006, 45, 7529-7543.	2.5	22
25	Aptamers targeting protein-specific glycosylation in tumor biomarkers: general selection, characterization and structural modeling. <i>Chemical Science</i> , 2020, 11, 9402-9413.	7.4	22
26	Application of the Interacting Quantum Atoms Approach to the S66 and Ionic-Hydrogen Bond Datasets for Noncovalent Interactions. <i>ChemPhysChem</i> , 2018, 19, 973-987.	2.1	21
27	Ammonolysis and Aminolysis of $\beta$ -Lactams: A Theoretical Study. <i>Chemistry - A European Journal</i> , 1999, 5, 1045-1054.	3.3	20
28	Quantum Chemical Study on the Coordination Environment of the Catalytic Zinc Ion in Matrix Metalloproteinases. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24222-24230.	2.6	19
29	From the X-ray Compact Structure to the Elongated Form of the Full-Length MMP-2 Enzyme in Solution: A Molecular Dynamics Study. <i>Journal of the American Chemical Society</i> , 2008, 130, 14070-14071.	13.7	19
30	Molecular dynamics simulations of the active matrix metalloproteinase-2: Positioning of the N-terminal fragment and binding of a small peptide substrate. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 72, 50-61.	2.6	18
31	Entropic Control of the Relative Stability of Triple-helical Collagen Peptide Models. <i>Journal of Physical Chemistry B</i> , 2008, 112, 15248-15255.	2.6	17
32	Conformational and entropy analyses of extended molecular dynamics simulations of $\alpha$ -, $\beta$ - and $\beta$ -cyclodextrins and of the $\beta$ -cyclodextrin/nabumetone complex. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1431-1440.	2.8	17
33	Affinity Calculations of Cyclodextrin Host-Guest Complexes: Assessment of Strengths and Weaknesses of End-Point Free Energy Methods. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 421-440.	5.4	17
34	NH <sub>3</sub> -Assisted Ammonolysis of $\beta$ -Lactams: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 1999, 64, 3281-3289.	3.2	16
35	Molecular Dynamics Simulations of Class C $\beta$ -Lactamase from <i>Citrobacter freundii</i> : Insights into the Base Catalyst for Acylation. <i>Biochemistry</i> , 2006, 45, 439-451.	2.5	16
36	Kinetic and binding effects in peptide substrate selectivity of matrix metalloproteinase-2: Molecular dynamics and QM/MM calculations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1-11.	2.6	16

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37	Evaluation of the Catalytic Mechanism of AICAR Transformylase by pH-Dependent Kinetics, Mutagenesis, and Quantum Chemical Calculations. <i>Journal of the American Chemical Society</i> , 2001, 123, 4687-4696.	13.7	15
38	Influence of charge configuration on substrate binding to SARS-CoV-2 main protease. <i>Chemical Communications</i> , 2021, 57, 5314-5317.	4.1	14
39	Water-Assisted Alkaline Hydrolysis of Monobactams: A Theoretical Study. <i>Chemistry - A European Journal</i> , 2002, 8, 859-867.	3.3	13
40	Assessing the Protonation State of Drug Molecules: The Case of Aztreonam. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 3235-3243.	6.4	13
41	Sampling Assessment for Molecular Simulations Using Conformational Entropy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4718-4729.	5.3	13
42	Fluorine conformational effects characterized by energy decomposition analysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 25258-25275.	2.8	13
43	Importance of a Synperiplanar Stepwise Mechanism through Neutral Intermediates in the Aminolysis of Monocyclic $\beta$ -Lactams: A Theoretical Analysis. <i>Journal of Organic Chemistry</i> , 1999, 64, 9144-9152.	3.2	11
44	Conformational properties of penicillins: Quantum chemical calculations and molecular dynamics simulations of benzylpenicillin. <i>Journal of Computational Chemistry</i> , 2003, 24, 1864-1873.	3.3	11
45	Understanding Regioselective Cleavage in Peptide Hydrolysis by a Palladium(II) Aqua Complex: A Theoretical Point of View. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8525-8535.	2.6	11
46	Zn <sup>2+</sup> -catalysed hydrolysis of $\beta$ -lactams: experimental and theoretical studies on the influence of the $\beta$ -lactam structure. <i>New Journal of Chemistry</i> , 2004, 28, 15-25.	2.8	10
47	Alkali and Alkaline Earth Cations in Complexes with Small Bioorganic Ligands: Ab Initio Benchmark Calculations and Bond Energy Decomposition. <i>ChemPhysChem</i> , 2020, 21, 99-112.	2.1	10
48	A Combined Theoretical and Experimental Research Project into the Aminolysis of $\beta$ -Lactam Antibiotics: The Importance of Bifunctional Catalysis. <i>European Journal of Organic Chemistry</i> , 2003, 2003, 4161-4172.	2.4	9
49	Strong <i>In Vitro</i> Activities of Two New Rifabutin Analogs against Multidrug-Resistant <i>Mycobacterium tuberculosis</i> . <i>Antimicrobial Agents and Chemotherapy</i> , 2010, 54, 5363-5365.	3.2	9
50	Role of the Protonation State on the Structure and Dynamics of Albumin. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1972-1988.	5.3	9
51	Ab Initio Benchmark Calculations on Ca(II) Complexes and Assessment of Density Functional Theory Methodologies. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11331-11343.	2.5	8
52	Alternative Interdomain Configurations of the Full-Length MMP-2 Enzyme Explored by Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2677-2686.	2.6	8
53	Ligand Strain and Entropic Effects on the Binding of Macrocyclic and Linear Inhibitors: Molecular Modeling of Penicillopepsin Complexes. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2045-2055.	5.4	7
54	Theoretical Study of the Reaction $1[:CH_2] + CHO + \hat{+} CH_3 + CO$ . <i>Journal of Physical Chemistry A</i> , 1998, 102, 9918-9924.	2.5	6

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55	Theoretical Study of Ammonolysis of Monobactams: Kinetic Role of the N-Sulfonate Group. <i>Helvetica Chimica Acta</i> , 2002, 85, 206-223.	1.6	6
56	Interdomain Conformations in the Full-Length MMP-2 Enzyme Explored by Protein-Protein Docking Calculations Using pyDock. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2204-2213.	5.3	6
57	Quantum chemical calculations of stability constants: study of ligand effects on the relative stability of Pd(II)-peptide complexes. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 465-475.	1.4	6
58	Unraveling the Molecular Structure of the Catalytic Domain of Matrix Metalloproteinase-2 in Complex with a Triple-Helical Peptide by Means of Molecular Dynamics Simulations. <i>Biochemistry</i> , 2013, 52, 8556-8569.	2.5	6
59	Amphiphilic cyclodextrins: Dimerization and diazepam binding explored by molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , 2022, 349, 118457.	4.9	6
60	QM/MM Energy Decomposition Using the Interacting Quantum Atoms Approach. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1510-1524.	5.4	6
61	Insights into the Base Catalysis Exerted by the DD-Transpeptidase from <i>Streptomyces</i> K15: A Molecular Dynamics Study. <i>Biochemistry</i> , 2005, 44, 3225-3240.	2.5	5
62	Extensive Simulations of the Full-Length Matrix Metalloproteinase-2 Enzyme in a Prereactive Complex with a Collagen Triple-Helical Peptide. <i>Biochemistry</i> , 2015, 54, 1243-1258.	2.5	5
63	Interacting Quantum Atoms Approach and Electrostatic Solvation Energy: Assessing Atomic and Group Solvation Contributions. <i>ChemPhysChem</i> , 2018, 19, 3425-3435.	2.1	5
64	Theoretical Study of Amine-Assisted Aminolysis of Penicillins - The Kinetic Role of the Carboxylate Group. <i>European Journal of Organic Chemistry</i> , 2001, 2001, 793-801.	2.4	4
65	Unraveling the distinctive features of hemorrhagic and non-hemorrhagic snake venom metalloproteinases using molecular simulations. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 69-83.	2.9	4
66	A combined semiempirical and DFT computational protocol for studying bioorganometallic complexes: Application to molybdocene-cysteine complexes. <i>Journal of Computational Chemistry</i> , 2014, 35, 324-334.	3.3	3
67	Molecular Modeling of Bioorganometallic Compounds: Thermodynamic Properties of Molybdocene-Glutathione Complexes and Mechanism of Peptide Hydrolysis. <i>ChemPhysChem</i> , 2015, 16, 1646-1656.	2.1	3
68	Molecular dynamics and quantum mechanical calculations on the mononuclear zinc-lactamase from <i>Bacillus cereus</i> : Protonation state of the active site and imipenem binding. <i>Computational and Theoretical Chemistry</i> , 2009, 912, 105-112.	1.5	2
69	Molecular Dynamics Studies of Matrix Metalloproteases. <i>Methods in Molecular Biology</i> , 2017, 1579, 111-134.	0.9	2
70	Understanding the Conformational Properties of Fluorinated Polypeptides: Molecular Modelling of Unguisin A. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 223-237.	5.4	2
71	Ring opening at N1-C2 bond of azetidin-2-ones by a molybdenum hydroxo-carbonyl complex: evidence from a computational study. <i>Dalton Transactions</i> , 2008, , 6427.	3.3	1
72	Ammonolysis and Aminolysis of -Lactams: A Theoretical Study. <i>Chemistry - A European Journal</i> , 1999, 5, 1045-1054.	3.3	0