Natalia Diaz

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7009110/publications.pdf

Version: 2024-02-01

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	Amphiphilic cyclodextrins: Dimerization and diazepam binding explored by molecular dynamics simulations. Journal of Molecular Liquids, 2022, 349, 118457.	4.9	6
2	QM/MM Energy Decomposition Using the Interacting Quantum Atoms Approach. Journal of Chemical Information and Modeling, 2022, 62, 1510-1524.	5.4	6
3	Understanding the Conformational Properties of Fluorinated Polypeptides: Molecular Modelling of Unguisin A. Journal of Chemical Information and Modeling, 2021, 61, 223-237.	5.4	2
4	Influence of charge configuration on substrate binding to SARS-CoV-2 main protease. Chemical Communications, 2021, 57, 5314-5317.	4.1	14
5	Alkali and Alkalineâ€Earth Cations in Complexes with Small Bioorganic Ligands: Abâ€…Initio Benchmark Calculations and Bond Energy Decomposition. ChemPhysChem, 2020, 21, 99-112.	2.1	10
6	Aptamers targeting protein-specific glycosylation in tumor biomarkers: general selection, characterization and structural modeling. Chemical Science, 2020, 11, 9402-9413.	7.4	22
7	SARS-CoV-2 Main Protease: A Molecular Dynamics Study. Journal of Chemical Information and Modeling, 2020, 60, 5815-5831.	5.4	112
8	Fluorine conformational effects characterized by energy decomposition analysis. Physical Chemistry Chemical Physics, 2019, 21, 25258-25275.	2.8	13
9	Affinity Calculations of Cyclodextrin Hostâ€“Guest Complexes: Assessment of Strengths and Weaknesses of End-Point Free Energy Methods. Journal of Chemical Information and Modeling, 2019, 59, 421-440.	5.4	17
10	Application of the Interacting Quantum Atoms Approach to the S66 and Ionicâ€Hydrogenâ€Bond Datasets for Noncovalent Interactions. ChemPhysChem, 2018, 19, 973-987.	2.1	21
11	Interacting Quantum Atoms Approach and Electrostatic Solvation Energy: Assessing Atomic and Group Solvation Contributions. ChemPhysChem, 2018, 19, 3425-3435.	2.1	5
12	Molecular Dynamics Studies of Matrix Metalloproteases. Methods in Molecular Biology, 2017, 1579, 111-134.	0.9	2
13	Conformational and entropy analyses of extended molecular dynamics simulations of Î±-, Î²- and Î³-cyclodextrins and of the Î²-cyclodextrin/nabumetone complex. Physical Chemistry Chemical Physics, 2017, 19, 1431-1440.	2.8	17
14	Ligand Strain and Entropic Effects on the Binding of Macrocyclic and Linear Inhibitors: Molecular Modeling of Penicillopepsin Complexes. Journal of Chemical Information and Modeling, 2017, 57, 2045-2055.	5.4	7
15	Role of the Protonation State on the Structure and Dynamics of Albumin. Journal of Chemical Theory and Computation, 2016, 12, 1972-1988.	5.3	9
16	Unraveling the distinctive features of hemorrhagic and non-hemorrhagic snake venom metalloproteinases using molecular simulations. Journal of Computer-Aided Molecular Design, 2016, 30, 69-83.	2.9	4
17	Molecular Modeling of Bioorganometallic Compounds: Thermodynamic Properties of Molybdoceneâ€“Glutathione Complexes and Mechanism of Peptide Hydrolysis. ChemPhysChem, 2015, 16, 1646-1656.	2.1	3
18	Extensive Simulations of the Full-Length Matrix Metalloproteinase-2 Enzyme in a Prereactive Complex with a Collagen Triple-Helical Peptide. Biochemistry, 2015, 54, 1243-1258.	2.5	5

#	Article	IF	Citations
19	Direct methods for computing singleâ€molecule entropies from molecular simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 1-26.	14.6	39
20	An Integrated Computational and Experimental Approach to Gaining Selectivity for MMPâ€2 within the Gelatinase Subfamily. ChemBioChem, 2014, 15, 399-412.	2.6	24
21	A combined semiempirical and DFT computational protocol for studying bioorganometallic complexes: Application to molybdoceneâ€“cysteine complexes. Journal of Computational Chemistry, 2014, 35, 324-334.	3.3	3
22	Sampling Assessment for Molecular Simulations Using Conformational Entropy Calculations. Journal of Chemical Theory and Computation, 2014, 10, 4718-4729.	5.3	13
23	Progress towards water-soluble triazole-based selective MMP-2 inhibitors. Organic and Biomolecular Chemistry, 2013, 11, 6623.	2.8	31
24	CENCALC: A computational tool for conformational entropy calculations from molecular simulations. Journal of Computational Chemistry, 2013, 34, 2041-2054.	3.3	32
25	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. Biochemistry, 2013, 52, 8556-8569.	2.5	6
26	Alternative Interdomain Configurations of the Full-Length MMP-2 Enzyme Explored by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 2677-2686.	2.6	8
27	Ab Initio Benchmark Calculations on Ca(II) Complexes and Assessment of Density Functional Theory Methodologies. Journal of Physical Chemistry A, 2011, 115, 11331-11343.	2.5	8
28	Entropy Calculations of Single Molecules by Combining the Rigidâ€“Rotor and Harmonic-Oscillator Approximations with Conformational Entropy Estimations from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2011, 7, 2638-2653.	5.3	56
29	Quantum chemical calculations of stability constants: study of ligand effects on the relative stability of Pd(II)â€“peptide complexes. Theoretical Chemistry Accounts, 2011, 128, 465-475.	1.4	6
30	Kinetic and binding effects in peptide substrate selectivity of matrix metalloproteinaseâ€2: Molecular dynamics and QM/MM calculations. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1-11.	2.6	16
31	Strong In Vitro Activities of Two New Rifabutin Analogs against Multidrug-Resistant Mycobacterium tuberculosis. Antimicrobial Agents and Chemotherapy, 2010, 54, 5363-5365.	3.2	9
32	Understanding Regioselective Cleavage in Peptide Hydrolysis by a Palladium(II) Aqua Complex: A Theoretical Point of View. Journal of Physical Chemistry B, 2010, 114, 8525-8535.	2.6	11
33	Interdomain Conformations in the Full-Length MMP-2 Enzyme Explored by Proteinâ^'Protein Docking Calculations Using pyDock. Journal of Chemical Theory and Computation, 2010, 6, 2204-2213.	5.3	6
34	Molecular dynamics and quantum mechanical calculations on the mononuclear zinc-Î²-lactamase from Bacillus cereus: Protonation state of the active site and imipenem binding. Computational and Theoretical Chemistry, 2009, 912, 105-112.	1.5	2
35	Thermochemical Fragment Energy Method for Biomolecules: Application to a Collagen Model Peptide. Journal of Chemical Theory and Computation, 2009, 5, 1667-1679.	5.3	37
36	Molecular dynamics simulations of the active matrix metalloproteinaseâ€2: Positioning of the Nâ€terminal fragment and binding of a small peptide substrate. Proteins: Structure, Function and Bioinformatics, 2008, 72, 50-61.	2.6	18

#	Article	IF	Citations
37	Ring opening at N1â€“C2 bond of azetidin-2-ones by a molybdenum hydroxo-carbonyl complex: evidence from a computational study. Dalton Transactions, 2008, , 6427.	3.3	1
38	Peptide Hydrolysis Catalyzed by Matrix Metalloproteinase 2: A Computational Study. Journal of Physical Chemistry B, 2008, 112, 8412-8424.	2.6	32
39	Entropic Control of the Relative Stability of Triple-helical Collagen Peptide Models. Journal of Physical Chemistry B, 2008, 112, 15248-15255.	2.6	17
40	From the X-ray Compact Structure to the Elongated Form of the Full-Length MMP-2 Enzyme in Solution: A Molecular Dynamics Study. Journal of the American Chemical Society, 2008, 130, 14070-14071.	13.7	19
41	Monoligand Zn(II) Complexes:â€‰ Ab Initio Benchmark Calculations and Comparison with Density Functional Theory Methodologies. Journal of Chemical Theory and Computation, 2008, 4, 243-256.	5.3	35
42	Molecular Dynamics Simulations of Matrix Metalloproteinase 2:â€‰ Role of the Structural Metal Ions[,]. Biochemistry, 2007, 46, 8943-8952.	2.5	37
43	A Computational Study of the Deacylation Mechanism of Human Butyrylcholinesterase. Biochemistry, 2006, 45, 7529-7543.	2.5	22
44	Molecular Dynamics Simulations of Class C Î²-Lactamase fromCitrobacter freundii:Â Insights into the Base Catalyst for Acylationâ€. Biochemistry, 2006, 45, 439-451.	2.5	16
45	Assessing the Protonation State of Drug Molecules:Â The Case of Aztreonam. Journal of Medicinal Chemistry, 2006, 49, 3235-3243.	6.4	13
46	Quantum Chemical Study on the Coordination Environment of the Catalytic Zinc Ion in Matrix Metalloproteinases. Journal of Physical Chemistry B, 2006, 110, 24222-24230.	2.6	19
47	Theoretical Studies on the Ring Opening of β-lactams: Processes in Solution and in Enzymatic Media. Current Organic Chemistry, 2006, 10, 805-821.	1.6	28
48	Molecular Dynamics Simulations of the TEM-1 Î²-Lactamase Complexed with Cephalothin. Journal of Medicinal Chemistry, 2005, 48, 780-791.	6.4	29
49	Insights into the Base Catalysis Exerted by the DD-Transpeptidase fromStreptomycesK15:Â A Molecular Dynamics Studyâ€. Biochemistry, 2005, 44, 3225-3240.	2.5	5
50	Zn2+catalysed hydrolysis of Î²-lactams: experimental and theoretical studies on the influence of the Î²-lactam structure. New Journal of Chemistry, 2004, 28, 15-25.	2.8	10
51	Insights into the Phosphoryl-Transfer Mechanism of cAMP-Dependent Protein Kinase from Quantum Chemical Calculations and Molecular Dynamics Simulations. Journal of the American Chemical Society, 2004, 126, 529-542.	13.7	67
52	Conformational properties of penicillins: Quantum chemical calculations and molecular dynamics simulations of benzylpenicillin. Journal of Computational Chemistry, 2003, 24, 1864-1873.	3.3	11
53	A Combined Theoretical and Experimental Research Project into the Aminolysis ofÎ²-Lactam Antibiotics: The Importance of Bifunctional Catalysis. European Journal of Organic Chemistry, 2003, 2003, 4161-4172.	2.4	9
54	Insights into the Acylation Mechanism of Class A Î²-Lactamases from Molecular Dynamics Simulations of the TEM-1 Enzyme Complexed with Benzylpenicillin. Journal of the American Chemical Society, 2003, 125, 672-684.	13.7	61

#	Article	IF	Citations
55	Ureases:â€‰ Quantum Chemical Calculations on Cluster Models. Journal of the American Chemical Society, 2003, 125, 15324-15337.	13.7	82
56	Water-Assisted Alkaline Hydrolysis of Monobactams: A Theoretical Study. Chemistry - A European Journal, 2002, 8, 859-867.	3.3	13
57	Theoretical Study of Ammonolysis of Monobactams: Kinetic Role of theN-Sulfonate Group. Helvetica Chimica Acta, 2002, 85, 206-223.	1.6	6
58	Molecular dynamics simulations of the dinuclear zinc-Î²-lactamase from Bacteroides fragilis complexed with imipenem. Journal of Computational Chemistry, 2002, 23, 1587-1600.	3.3	52
59	Molecular Dynamics Study of the IIA Binding Site in Human Serum Albumin:Â Influence of the Protonation State of Lys195 and Lys199. Journal of Medicinal Chemistry, 2001, 44, 250-260.	6.4	74
60	A Theoretical Study of the Aminolysis Reaction of Lysine 199 of Human Serum Albumin with Benzylpenicillin:Â Consequences for Immunochemistry of Penicillins. Journal of the American Chemical Society, 2001, 123, 7574-7583.	13.7	23
61	Acylation of Class A Î²-lactamases by Penicillins:â€‰ A Theoretical Examination of the Role of Serine 130 and the Î²-lactam Carboxylate Group. Journal of Physical Chemistry B, 2001, 105, 11302-11313.	2.6	42
62	Molecular Dynamics Simulations of the Mononuclear Zinc-Î²-lactamase fromBacilluscereusComplexed with Benzylpenicillin and a Quantum Chemical Study of the Reaction Mechanism. Journal of the American Chemical Society, 2001, 123, 9867-9879.	13.7	66
63	Evaluation of the Catalytic Mechanism of AICAR Transformylase by pH-Dependent Kinetics, Mutagenesis, and Quantum Chemical Calculations. Journal of the American Chemical Society, 2001, 123, 4687-4696.	13.7	15
64	Theoretical Study of Amine-Assisted Aminolysis of Penicillins â^' The Kinetic Role of the Carboxylate Group. European Journal of Organic Chemistry, 2001, 2001, 793-801.	2.4	4
65	Hydration of zinc ions: theoretical study of [Zn(H2O)4](H2O)82+ and [Zn(H2O)6](H2O)62+. Chemical Physics Letters, 2000, 326, 288-292.	2.6	45
66	Theoretical Study of the Water-Assisted Aminolysis of Î²-Lactams:Â Implications for the Reaction between Human Serum Albumin and Penicillins. Journal of the American Chemical Society, 2000, 122, 6710-6719.	13.7	29
67	Zinc Metallo-Î²-Lactamase from Bacteroides fragilis:â€‰ A Quantum Chemical Study on Model Systems of the Active Site. Journal of the American Chemical Society, 2000, 122, 4197-4208.	13.7	84
68	Ammonolysis and Aminolysis ofÎ²-Lactams: A Theoretical Study. Chemistry - A European Journal, 1999, 5, 1045-1054.	3.3	20
69	NH3-Assisted Ammonolysis of Î²-Lactams:Â A Theoretical Study. Journal of Organic Chemistry, 1999, 64, 3281-3289.	3.2	16
70	Importance of a Synperiplanar Stepwise Mechanism through Neutral Intermediates in the Aminolysis of Monocyclic Î²-Lactams:Â A Theoretical Analysis. Journal of Organic Chemistry, 1999, 64, 9144-9152.	3.2	11
71	Ammonolysis and Aminolysis of -Lactams: A Theoretical Study. Chemistry - A European Journal, 1999, 5, 1045-1054.	3.3	0
72	Theoretical Study of the Reaction 1[:CH2] + CHO+ â†' CH3+ + CO. Journal of Physical Chemistry A, 1998, 102, 9918-9924.	2.5	6