Marco D'Abramo

List of Publications by Year
in descending order

85	1,594	279487 23	344852 36
papers	citations	h-index	g-index

88	88	88	1974
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	MoDEL (Molecular Dynamics Extended Library): AÂDatabase of Atomistic Molecular Dynamics Trajectories. Structure, 2010, 18, 1399-1409.	1.6	123
2	FlexServ: an integrated tool for the analysis of protein flexibility. Bioinformatics, 2009, 25, 1709-1710.	1.8	72
3	Theoretical characterization of electronic states in interacting chemical systems. Journal of Chemical Physics, 2009, 130, 084109.	1.2	66
4	Structural Characterization of Proteinâ€“Protein Complexes by Integrating Computational Docking with Small-angle Scattering Data. Journal of Molecular Biology, 2010, 403, 217-230.	2.0	64
5	Molecular basis of engineered meganuclease targeting of the endogenous human RAG1 locus. Nucleic Acids Research, 2011, 39, 729-743.	6.5	63
6	Comparing the Efficiency of Biased and Unbiased Molecular Dynamics in Reconstructing the Free Energy Landscape of Met-Enkephalin. Journal of Chemical Theory and Computation, 2010, 6, 3640-3646.	2.3	51
7	Extending the perturbed matrix method beyond the dipolar approximation: comparison of different levels of theory. Physical Chemistry Chemical Physics, 2018, 20, 24369-24378.	1.3	49
8	Electronic properties of formaldehyde in water: a theoretical study. Chemical Physics Letters, 2003, 381, 187-193.	1.2	46
9	On the Nature of DNA Hyperchromic Effect. Journal of Physical Chemistry B, 2013, 117, 8697-8704.	1.2	44
10	Theoretical Characterization of Î±-Helix and Î²-Hairpin Folding Kinetics. Journal of the American Chemical Society, 2005, 127, 14825-14832.	6.6	43
11	Theoretical modeling of UV-Vis absorption and emission spectra in liquid state systems including vibrational and conformational effects: Explicit treatment of the vibronic transitions. Journal of Chemical Physics, 2014, 140, 164104.	1.2	42
12	Theoretical Characterization of the Dynamical Behavior and Transport Properties of Î±,Î³-Peptide Nanotubes in Solution. Journal of the American Chemical Society, 2009, 131, 15678-15686.	6.6	41
13	The p53 tetramer shows an induced-fit interaction of the C-terminal domain with the DNA-binding domain. Oncogene, 2016, 35, 3272-3281.	2.6	40
14	Theoretical modeling of the valence UV spectra of 1,2,3-triazine and uracil in solution. Physical Chemistry Chemical Physics, 2006, 8, 1385.	1.3	39
15	Mixed Quantum-Classical Methods for Molecular Simulations of Biochemical Reactions With Microwave Fields: The Case Study of Myoglobin. IEEE Transactions on Microwave Theory and Techniques, 2008, 56, 2511-2519.	2.9	36
16	In silico characterization of protein partial molecular volumes and hydration shells. Physical Chemistry Chemical Physics, 2015, 17, 31270-31277.	1.3	35
17	Theoretical modeling of vibroelectronic quantum states in complex molecular systems: Solvated carbon monoxide, a test case. Journal of Chemical Physics, 2005, 122, 124506.	1.2	34
18	Theoretical Characterisation of the Electronic Excitation in Liquid Water. ChemPhysChem, 2005, 6, 53-58.	1.0	31

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19	Theoretical modeling of chemical reactions in complex environments: the intramolecular proton transfer in aqueous malonaldehyde. Journal of Physical Organic Chemistry, 2006, 19, 518-530.	0.9	28
20	Conformational behavior of temporin A and temporin L in aqueous solution: A computational/experimental study. Biopolymers, 2006, 81, 215-224.	1.2	28
21	Statistical mechanical modelling of chemical reactions in complex systems: the kinetics of the Haem carbon monoxide bindingâ€“unbinding reaction in Myoglobin. Theoretical Chemistry Accounts, 2007, 117, 637-647.	0.5	28
22	Molecular dynamics of the full-length p53 monomer. Cell Cycle, 2013, 12, 3098-3108.	1.3	27
23	Non-specific proteinâ€“DNA interactions control I-CreI target binding and cleavage. Nucleic Acids Research, 2012, 40, 6936-6945.	6.5	24
24	Theoretical characterization of temperature and density dependence of liquid water electronic excitation energy: Comparison with recent experimental data. Journal of Chemical Physics, 2008, 128, 021103.	1.2	22
25	Exploiting Reactionâ€Diffusion Conditions to Trigger Pathway Complexity in the Growth of a MOF. Angewandte Chemie - International Edition, 2021, 60, 15920-15927.	7.2	19
26	Statistical Mechanics and Thermodynamics of Simulated Ionic Solutions. Journal of Physical Chemistry B, 2002, 106, 11843-11848.	1.2	18
27	Characterization of the catalytic flexible loop in the dihydroorotase domain of the human multi-enzymatic protein CAD. Journal of Biological Chemistry, 2018, 293, 18903-18913.	1.6	18
28	Molecular Dynamics Simulations Reveal Canonical Conformations in Different pMHC/TCR Interactions. Cells, 2020, 9, 942.	1.8	18
29	Kinetics of Carbon Monoxide Migration and Binding in Solvated Myoglobin as Revealed by Molecular Dynamics Simulations and Quantum Mechanical Calculations. Journal of Physical Chemistry B, 2009, 113, 16346-16353.	1.2	17
30	Equilibrium between 5- and 6-Fold Coordination in the First Hydration Shell of Cu(II). Journal of Physical Chemistry A, 2016, 120, 3958-3965.	1.1	17
31	Quantitative Characterization of Binding Pockets and Binding Complementarity by Means of Zernike Descriptors. Journal of Chemical Information and Modeling, 2020, 60, 1390-1398.	2.5	17
32	Conformational Selection versus Induced Fit in Kinases: The Case of PI3Kâ€Î³. Angewandte Chemie - International Edition, 2012, 51, 642-646.	7.2	16
33	The self-association equilibria of doxorubicin at high concentration and ionic strength characterized by fluorescence spectroscopy and molecular dynamics simulations. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2019, 577, 517-522.	2.3	16
34	Theoretical-computational modeling of photo-induced charge separation spectra and charge recombination kinetics in solution. Physical Chemistry Chemical Physics, 2014, 16, 20624-20638.	1.3	15
35	Photoinduced electron transfer in a dichromophoric peptide: a numerical experiment. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	14
36	Molecular mechanisms of activation in CDK2. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1929-1935.	2.0	13

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37	Theoretical Characterization of the Reduction Potentials of Nucleic Acids in Solution. Journal of Chemical Theory and Computation, 2021, 17, 1301-1307.	2.3	13
38	Theoretical study of intramolecular charge transfer in Ï€-conjugated oligomers. Chemical Physics Letters, 2007, 434, 194-199.	1.2	12
39	Modeling conformational transitions in kinases by molecular dynamics simulations: achievements, difficulties, and open challenges. Frontiers in Genetics, 2014, 5, 128.	1.1	12
40	Theoretical calculation of the pyrene emission properties in different solvents. Chemical Physics Letters, 2015, 639, 17-22.	1.2	12
41	Understanding the indirect DNA read-out specificity of I-CreI Meganuclease. Scientific Reports, 2018, 8, 10286.	1.6	12
42	Role of the hydrophilic spacer of glucosylated amphiphiles included in liposome formulations in the recognition of Concanavalin A. Colloids and Surfaces B: Biointerfaces, 2015, 136, 232-239.	2.5	11
43	A Stereochemically Driven Supramolecular Polymerisation. Chemistry - A European Journal, 2018, 24, 8195-8204.	1.7	11
44	Unusual Placement of an EBV Epitope into the Groove of the Ankylosing Spondylitis-Associated HLA-B27 Allele Allows CD8+ T Cell Activation. Cells, 2019, 8, 572.	1.8	11
45	Density discriminates between thermophilic and mesophilic proteins. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3265-3273.	2.0	10
46	Molecular Dynamics Study of Naturally Existing Cavity Couplings in Proteins. PLoS ONE, 2015, 10, e0119978.	1.1	10
47	On the use of the quasi-Gaussian entropy theory in the study of simulated dilute solutions. Journal of Chemical Physics, 2004, 120, 5226-5234.	1.2	9
48	Kinetics and mechanistic study of competitive inhibition of thymidine phosphorylase by 5-fluoruracil derivatives. Colloids and Surfaces B: Biointerfaces, 2016, 140, 121-127.	2.5	9
49	Key Players in I-DmoI Endonuclease Catalysis Revealed from Structure and Dynamics. ACS Chemical Biology, 2016, 11, 1401-1407.	1.6	9
50	Conformational Mobility and Efficiency in Supramolecular Catalysis. A Computational Approach to Evaluate the Performances of Enzyme Mimics. European Journal of Organic Chemistry, 2020, 2020, 6004-6011.	1.2	9
51	Insights into the Interaction Mechanism of DTP3 with MKK7 by Using STD-NMR and Computational Approaches. Biomedicines, 2021, 9, 20.	1.4	9
52	Electric-driven membrane poration: A rationale for water role in the kinetics of pore formation. Bioelectrochemistry, 2022, 143, 107987.	2.4	9
53	Theoretical Modeling of Redox Potentials of Biomolecules. Molecules, 2022, 27, 1077.	1.7	9
54	Absorption behavior of doxorubicin hydrochloride in visible region in different environments: a combined experimental and computational study. Physical Chemistry Chemical Physics, 2022, 24, 12027-12035.	1.3	9

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55	Effects of local electric fields on the redox free energy of single stranded DNA. Chemical Communications, 2011, 47, 2646-2648.	2.2	8
56	Myoglobin as a Case Study for Molecular Simulations in the Presence of a Microwave Electromagnetic Field. , 2006, , .		7
57	Intramolecular charge transfer in ï€-conjugated oligomers: a theoretical study on the effect of temperature and oxidation state. Theoretical Chemistry Accounts, 2008, 119, 469-476.	0.5	7
58	On the Use of low-resolution Data to Improve Structure Prediction of Proteins and Protein Complexes. Journal of Chemical Theory and Computation, 2009, 5, 3129-3137.	2.3	7
59	Charge transfer equilibria of aqueous single stranded DNA. Physical Chemistry Chemical Physics, 2009, 11, 10614.	1.3	7
60	Engineering a Nickase on the Homing Endonuclease I-DmoI Scaffold. Journal of Biological Chemistry, 2015, 290, 18534-18544.	1.6	7
61	Efficient and Accurate Modeling of Conformational Transitions in Proteins: The Case of c-Src Kinase. Journal of Physical Chemistry B, 2018, 122, 8853-8860.	1.2	7
62	DNA cleavage by endonuclease I-DmoI: a QM/MM study and comparison with experimental data provide indications on the environmental effects. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	7
63	Calculation of the optical rotatory dispersion of solvated alanine by means of the perturbed matrix method. Chemical Physics Letters, 2005, 402, 559-563.	1.2	6
64	Ground and excited electronic state thermodynamics of aqueous carbon monoxide: A theoretical study. Journal of Chemical Physics, 2005, 122, 124507.	1.2	6
65	On the activation and deactivation pathways of the Lck kinase domain: a computational study. Journal of Computer-Aided Molecular Design, 2019, 33, 597-603.	1.3	6
66	Point Mutations at a Key Site Alter the Cytochrome P450 OleP Structural Dynamics. Biomolecules, 2022, 12, 55.	1.8	6
67	On the importance of configurational sampling in theoretical calculation of electronic properties of complex molecular systems: Acetone in water. Chemical Physics Letters, 2006, 424, 289-294.	1.2	5
68	2â€(Hydroxyimino)aldehydes: Photoâ€•and Physicochemical Properties of a Versatile Functional Group for Monomer Design. Chemistry - A European Journal, 2018, 24, 7683-7694.	1.7	5
69	Rationalizing Sequence and Conformational Effects on the Guanine Oxidation in Different DNA Conformations. Journal of Physical Chemistry B, 2022, 126, 5017-5023.	1.2	5
70	Theoreticalâ€“computational modelling of the temperature dependence of the foldingâ€“unfolding thermodynamics and kinetics: the case of a Trp-cage. Physical Chemistry Chemical Physics, 2019, 21, 23162-23168.	1.3	4
71	C-12 vs C-3 substituted bile salts: An example of the effects of substituent position and orientation on the self-assembly of steroid surfactant isomers. Colloids and Surfaces B: Biointerfaces, 2020, 185, 110556.	2.5	4
72	Quaternary Structure Transitions of Human Hemoglobin: An Atomic-Level View of the Functional Intermediate States. Journal of Chemical Information and Modeling, 2021, 61, 3988-3999.	2.5	4

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73	Theoretical prediction of thermodynamic equilibrium constants of chemical reactions in water. Computational and Theoretical Chemistry, 2007, 811, 197-201.	1.5	3
74	What can we learn by comparing experimental and theoretical-computational X-ray scattering data?. Journal of Molecular Liquids, 2009, 144, 9-12.	2.3	3
75	Computational Modeling of the Thermodynamics of the Mesophilic and Thermophilic Mutants of Trp-Cage Miniprotein. ACS Omega, 2022, 7, 13448-13454.	1.6	3
76	Characterization of liquid behaviour by means of local density fluctuations. Journal of Molecular Liquids, 2005, 117, 17-21.	2.3	2
77	Structure and dynamics of mesophilic variants from the homing endonuclease I-DmoI. Journal of Computer-Aided Molecular Design, 2017, 31, 1063-1072.	1.3	2
78	Modelling the Activation Pathways in Full-Length Src Kinase. Biophysica, 2021, 1, 238-248.	0.6	2
79	The Full Model of the pMHC-TCR-CD3 Complex: A Structural and Dynamical Characterization of Bound and Unbound States. Cells, 2022, 11, 668.	1.8	2
80	Effect of DNA on the conformational dynamics of the endonucleases Iâ€Ðmol as provided by molecular dynamics simulations. Biopolymers, 2016, 105, 898-904.	1.2	1
81	Investigating the oxidative refolding mechanism of Cripto-1 CFC domain. International Journal of Biological Macromolecules, 2019, 137, 1179-1189.	3.6	1
82	Evolutionary Modes in Protein Observable Space: The Case of Thioredoxins. Journal of Molecular Evolution, 2019, 87, 175-183.	0.8	1
83	Exploiting Reactionâ€Ðiffusion Conditions to Trigger Pathway Complexity in the Growth of a MOF. Angewandte Chemie, 2021, 133, 16056-16063.	1.6	1
84	Theoretical Study of the Thermodynamics of a Solvated Peptide: Contryphan Vn. Physica Scripta, 2005, , 196.	1.2	1
85	Innentitelbild: Exploiting Reactionâ€Ðiffusion Conditions to Trigger Pathway Complexity in the Growth of a MOF (Angew. Chem. 29/2021). Angewandte Chemie, 2021, 133, 15794-15794.	1.6	0