Alfredo Di Nola

List of Publications by Year
in descending order

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70	2,729	147726	197736
papers	citations	31 h-index	49 g-index

70	70	70	2594
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Kinetics of Carbon Monoxide Migration and Binding in Solvated Neuroglobin As Revealed by Molecular Dynamics Simulations and Quantum Mechanical Calculations. Journal of Physical Chemistry B, 2011, 115, 2436-2446.	1.2	17
2	Molecular Origin of Gerstmann-StrÃussler-Scheinker Syndrome: Insight from Computer Simulation of an Amyloidogenic Prion Peptide. Biophysical Journal, 2011, 100, 3000-3007.	0.2	11
3	Analysis of Infrared Spectra of Î²-Hairpin Peptides As Derived from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 11872-11878.	1.2	11
4	Structure of the lipodepsipeptide syringomycin E in phospholipids and sodium dodecylsulphate micelle studied by circular dichroism, NMR spectroscopy and molecular dynamics. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 2102-2110.	1.4	15
5	The effects of the L29F mutation on the ligand migration kinetics in crystallized myoglobin as revealed by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2011, 79, 867-879.	1.5	4
6	Theoretical-computational modelling of infrared spectra in peptides and proteins: a new frontier for combined theoretical-experimental investigations. Current Opinion in Structural Biology, 2010, 20, 155-161.	2.6	35
7	On the origin of IR spectral changes upon protein folding. Chemical Physics Letters, 2010, 488, 213-218.	1.2	30
8	Free-Energy Profile for CO Binding to Separated Chains of Human and Trematomus newnesi Hemoglobin: Insights from Molecular Dynamics Simulations and Perturbed Matrix Method. Journal of Physical Chemistry B, 2010, 114, 7002-7008.	1.2	7
9	Dynamic Investigation of Protein Metal Active Sites: Interplay of XANES and Molecular Dynamics Simulations. Journal of the American Chemical Society, 2010, 132, 14901-14909.	6.6	18
10	Structural, thermodynamic, and kinetic properties of Gramicidin analogue GS6 studied by molecular dynamics simulations and statistical mechanics. Biopolymers, 2009, 91, 1154-1160.	1.2	1
11	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
12	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
13	The Kinetics of Ligand Migration in Crystallized Myoglobin as Revealed by Molecular Dynamics Simulations. Biophysical Journal, 2008, 94, 4277-4281.	0.2	31
14	Molecular Dynamics Simulation of the Neuroglobin Crystal: Comparison with the Simulation in Solution. Biophysical Journal, 2008, 95, 4157-4162.	0.2	26
15	Molecular dynamics simulation of the interaction between the complex iron-sulfur flavoprotein glutamate synthase and its substrates. Protein Science, 2008, 13, 2979-2991.	3.1	8
16	Solvent Electrostriction-Driven Peptide Folding Revealed by Quasi-Gaussian Entropy Theory and Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 11155-11163.	1.2	9
17	Protein Folding Pathways Revealed by Essential Dynamics Sampling. Journal of Chemical Theory and Computation, 2008, 4, 1940-1948.	2.3	13
18	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

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19	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
20	Statistical Mechanical Modeling of Chemical Reactions in Condensed Phase Systems. Challenges and Advances in Computational Chemistry and Physics, 2008, , 191-213.	0.6	9
21	Dehydration-driven solvent exposure of hydrophobic surfaces as a driving force in peptide folding. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 15230-15235.	3.3	72
22	A Generalized Born Implicit-Membrane Representation Compared to Experimental Insertion Free Energies. Biophysical Journal, 2007, 92, 2338-2349.	0.2	74
23	Theoretical Characterization of Carbon Monoxide Vibrational Spectrum in Sperm Whale Myoglobin Distal Pocket. Biophysical Journal, 2007, 92, 3442-3447.	0.2	23
24	Molecular Dynamics Simulation of Deoxy and Carboxy Murine Neuroglobin in Water. Biophysical Journal, 2007, 93, 434-441.	0.2	42
25	Theoretical study of intramolecular charge transfer in Ï€-conjugated oligomers. Chemical Physics Letters, 2007, 434, 194-199.	1.2	12
26	Monte carlo folding of trans-membrane helical peptides in an implicit generalized Born membrane. Proteins: Structure, Function and Bioinformatics, 2007, 69, 297-308.	1.5	21
27	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
28	Myoglobin as a Case Study for Molecular Simulations in the Presence of a Microwave Electromagnetic Field. , 2006, , .		7
29	Monte Carlo vs Molecular Dynamics for All-Atom Polypeptide Folding Simulations. Journal of Physical Chemistry B, 2006, 110, 16733-16742.	1.2	49
30	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
31	Evaluating Tilt Angles of Membrane-Associated Helices: Comparison of Computational and NMR Techniques. Biophysical Journal, 2006, 90, 1650-1660.	0.2	54
32	On the Effect of a Point Mutation on the Reactivity of CuZn Superoxide Dismutase:Â A Theoretical Study. Journal of Physical Chemistry B, 2006, 110, 7538-7544.	1.2	16
33	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
34	Aggregation of small peptides studied by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2006, 65, 914-921.	1.5	19
35	Theoretical Characterisation of the Electronic Excitation in Liquid Water. ChemPhysChem, 2005, 6, 53-58.	1.0	31
36	Properties of integral membrane protein structures: Derivation of an implicit membrane potential. Proteins: Structure, Function and Bioinformatics, 2005, 59, 252-265.	1.5	174

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37	Molecular dynamics simulation of the aggregation of the core-recognition motif of the islet amyloid polypeptide in explicit water. Proteins: Structure, Function and Bioinformatics, 2005, 59, 519-527.	1.5	49
38	Thermodynamic and kinetic characterization of a Î²-hairpin peptide in solution: An extended phase space sampling by molecular dynamics simulations in explicit water. Proteins: Structure, Function and Bioinformatics, 2005, 59, 510-518.	1.5	49
39	Misfolding of the amyloid Î²-protein: A molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2005, 62, 183-192.	1.5	55
40	Ground and excited electronic state thermodynamics of aqueous carbon monoxide: A theoretical study. Journal of Chemical Physics, 2005, 122, 124507.	1.2	6
41	Theoretical Characterization of Î±-Helix and Î²-Hairpin Folding Kinetics. Journal of the American Chemical Society, 2005, 127, 14825-14832.	6.6	43
42	Molecular Dynamics Simulation of Sperm Whale Myoglobin: Effects of Mutations and Trapped CO on the Structure and Dynamics of Cavities. Biophysical Journal, 2005, 89, 465-474.	0.2	93
43	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
44	Î²-Hairpin conformation of fibrillogenic peptides: Structure and Î±-Î² transition mechanism revealed by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2004, 57, 198-204.	1.5	85
45	A molecular dynamics study of acylphosphatase in aggregation-promoting conditions: The influence of trifluoroethanol/water solvent. Biopolymers, 2004, 75, 491-496.	1.2	4
46	Conformational fluctuations and electronic properties in myoglobin. Journal of Computational Chemistry, 2004, 25, 974-984.	1.5	35
47	Theoretical Modeling of Enzyme Reaction Chemistry:Â The Electron Transfer of the Reduction Mechanism in CuZn Superoxide Dismutase. Journal of Physical Chemistry B, 2004, 108, 16255-16260.	1.2	31
48	Extended Molecular Dynamics Simulation of the Carbon Monoxide Migration in Sperm Whale Myoglobin. Biophysical Journal, 2004, 86, 3855-3862.	0.2	129
49	The Effect of Protein Conformational Flexibility on the Electronic Properties of a Chromophore. Biophysical Journal, 2003, 84, 2805-2813.	0.2	36
50	Molecular Dynamics Simulation of Protein Folding by Essential Dynamics Sampling: Folding Landscape of Horse Heart Cytochrome c. Biophysical Journal, 2003, 85, 2865-2871.	0.2	67
51	Selective Excitation of Native Fluctuations during Thermal Unfolding Simulations: Horse Heart Cytochrome c as a Case Study. Biophysical Journal, 2003, 84, 1876-1883.	0.2	45
52	Global and local motions in ribonuclease A: A molecular dynamics study. Biopolymers, 2002, 65, 274-283.	1.2	56
53	Molecular dynamics study of a hyperthermophilic and a mesophilic rubredoxin. Proteins: Structure, Function and Bioinformatics, 2002, 46, 287-294.	1.5	58
54	Dynamic effects of mutations within two loops of cytochrome c551 from Pseudomonas aeruginosa. Proteins: Structure, Function and Bioinformatics, 2002, 50, 222-229.	1.5	20

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55	Extension of the perturbed matrix method: application to a water molecule. Chemical Physics Letters, 2002, 365, 450-456.	1.2	51
56	Computational study of the catalytic domain of human neutrophil collagenase. specific role of the S3 and S'3 subsites in the interaction with a phosphonate inhibitor. Journal of Computer-Aided Molecular Design, 2002, 16, 213-225.	1.3	13
57	On the Use of the Quasi-Gaussian Entropy Theory in Systems of Polyatomic Flexible Molecules. Journal of Physical Chemistry B, 2001, 105, 1834-1844.	1.2	8
58	Conformations in solution of the fuscopeptins. Phytotoxic metabolites of Pseudomonas fuscovaginae. FEBS Journal, 1999, 266, 484-492.	0.2	12
59	A molecular dynamics study of the 41â€56 Î²â€hairpin from B1 domain of protein G. Protein Science, 1999, 8, 2130-2143.	3.1	109
60	Docking of flexible ligands to flexible receptors in solution by molecular dynamics simulation. , 1999, 35, 153-162.		118
61	On the convergence of the conformational coordinates basis set obtained by the essential dynamics analysis of proteins' molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 1999, 36, 419-424.	1.5	277
62	Effects of core-packing on the structure, function, and mechanics of a four-helix-bundle protein ROP. Proteins: Structure, Function and Bioinformatics, 1999, 36, 436-446.	1.5	12
63	Mechanics and dynamics of B1 domain of protein G: Role of packing and surface hydrophobic residues. Protein Science, 1999, 8, 147-160.	3.1	46
64	On the convergence of the conformational coordinates basis set obtained by the essential dynamics analysis of proteins' molecular dynamics simulations. , 1999, 36, 419.		1
65	On the convergence of the conformational coordinates basis set obtained by the essential dynamics analysis of proteins' molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 1999, 36, 419-424.	1.5	8
66	Solution conformation of the Pseudomonas syringae MSU 16H phytotoxic lipodepsipeptide Pseudomycin A determined by computer simulations using distance geometry and molecular dynamics from NMR data. FEBS Journal, 1998, 257, 449-456.	0.2	9
67	Free energy calculations in globular proteins: Methods to reduce errors. Journal of Computational Chemistry, 1998, 19, 1229-1240.	1.5	6
68	Solution Conformation of the Pseudomonas Syringae Pv. Syringae Phytotoxic Lipodepsipeptide Syringopeptin 25-A. Two-Dimensional NMR, Distance Geometry and Molecular Dynamics. FEBS Journal, 1995, 234, 747-758.	0.2	33
69	Determination of structure and conformation in solution of syringotoxin, a lipodepsipeptide fromPseudomonas syringae pv.syringae by 2D NMR and molecular dynamics. Structural Chemistry, 1994, 5, 43-50.	1.0	19
70	Molecular dynamics simulation of the docking of substrates to proteins. Proteins: Structure, Function and Bioinformatics, 1994, 19, 174-182.	1.5	96