

Danilo Roccatano

List of Publications by Year in descending order

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96
papers

3,997
citations

94433

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133252

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98
docs citations

98
times ranked

4602
citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanism by which 2,2,2-trifluoroethanol/water mixtures stabilize secondary-structure formation in peptides: A molecular dynamics study. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 12179-12184.	7.1	465
2	An extended x-ray absorption fine structure study of aqueous solutions by employing molecular dynamics simulations. Journal of Chemical Physics, 1994, 100, 985-994.	3.0	133
3	A Statistical Analysis of Random Mutagenesis Methods Used for Directed Protein Evolution. Journal of Molecular Biology, 2006, 355, 858-871.	4.2	132
4	Extended Molecular Dynamics Simulation of the Carbon Monoxide Migration in Sperm Whale Myoglobin. Biophysical Journal, 2004, 86, 3855-3862.	0.5	129
5	Docking of flexible ligands to flexible receptors in solution by molecular dynamics simulation. , 1999, 35, 153-162.		118
6	A molecular dynamics study of the 41-56 β -hairpin from B1 domain of protein G. Protein Science, 1999, 8, 2130-2143.	7.6	109
7	A New 2,2,2-Trifluoroethanol Model for Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2000, 104, 12347-12354.	2.6	106
8	Molecular dynamics simulation of the docking of substrates to proteins. Proteins: Structure, Function and Bioinformatics, 1994, 19, 174-182.	2.6	96
9	A 10-Å... Spectroscopic Ruler Applied to Short Polyprolines. Journal of the American Chemical Society, 2007, 129, 9762-9772.	13.7	87
10	Structural flexibility of the nucleosome core particle at atomic resolution studied by molecular dynamics simulation. Biopolymers, 2007, 85, 407-421.	2.4	86
11	β -Hairpin conformation of fibrillogenic peptides: Structure and β - β transition mechanism revealed by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2004, 57, 198-204.	2.6	85
12	Understanding the Interaction of Block Copolymers with DMPC Lipid Bilayer Using Coarse-Grained Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 14333-14345.	2.6	77
13	Effect of hexafluoroisopropanol alcohol on the structure of melittin: A molecular dynamics simulation study. Protein Science, 2005, 14, 2582-2589.	7.6	76
14	Modular assembly of proteins on nanoparticles. Nature Communications, 2018, 9, 1489.	12.8	76
15	Model of 1,1,1,3,3,3-Hexafluoro-propan-2-ol for Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2001, 105, 10967-10975.	2.6	72
16	Distance Distributions of Short Polypeptides Recovered by Fluorescence Resonance Energy Transfer in the 10 Å... Domain. Journal of the American Chemical Society, 2006, 128, 8118-8119.	13.7	68
17	Laboratory evolution of P450 BM3 for mediated electron transfer yielding an activity-improved and reductase-independent variant. Protein Engineering, Design and Selection, 2007, 21, 29-35.	2.1	68
18	Molecular Dynamics Simulation of Protein Folding by Essential Dynamics Sampling: Folding Landscape of Horse Heart Cytochrome c. Biophysical Journal, 2003, 85, 2865-2871.	0.5	67

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19	Directed evolution of a highly active <i>Yersinia mollaretii</i> phytase. <i>Applied Microbiology and Biotechnology</i> , 2012, 95, 405-418.	3.6	64
20	Functionalized Nanocompartments (Synthosomes) with a Reduction-Triggered Release System. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 7029-7031.	13.8	63
21	Steering directed protein evolution: strategies to manage combinatorial complexity of mutant libraries. <i>Environmental Microbiology</i> , 2007, 9, 2645-2659.	3.8	59
22	Molecular dynamics simulation study of solvent effects on conformation and dynamics of polyethylene oxide and polypropylene oxide chains in water and in common organic solvents. <i>Journal of Chemical Physics</i> , 2012, 136, 124901.	3.0	59
23	Hybrid Particle-Field Coarse-Grained Models for Biological Phospholipids. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2947-2962.	5.3	58
24	COMPUTER-AIDED PROTEIN DIRECTED EVOLUTION: A REVIEW OF WEB SERVERS, DATABASES AND OTHER COMPUTATIONAL TOOLS FOR PROTEIN ENGINEERING. <i>Computational and Structural Biotechnology Journal</i> , 2012, 2, e201209008.	4.1	52
25	Folding and stability of the three-stranded β -sheet peptide Betanova: Insights from molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002, 46, 380-392.	2.6	50
26	Interaction of Curcumin with PEO- <i>b</i> -PPO- <i>b</i> -PEO Block Copolymers: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3250-3257.	2.6	50
27	Multielectron excitations at the Ledges of barium in aqueous solution. <i>Physical Review B</i> , 1996, 54, 12129-12138.	3.2	48
28	Structure and Dynamics of Dodecaborate Clusters in Water. <i>Inorganic Chemistry</i> , 2012, 51, 4894-4896.	4.0	47
29	Sensitive Assay for Laboratory Evolution of Hydroxylases toward Aromatic and Heterocyclic Compounds. <i>Journal of Biomolecular Screening</i> , 2005, 10, 246-252.	2.6	46
30	Ionic liquid effects on the activity of monooxygenase P450 BM-3. <i>Green Chemistry</i> , 2008, 10, 117-123.	9.0	46
31	Assessment of the validity of intermolecular potential models used in molecular dynamics simulations by extended x-ray absorption fine structure spectroscopy: A case study of Sr ²⁺ in methanol solution. <i>Journal of Chemical Physics</i> , 1998, 108, 9487-9497.	3.0	45
32	Investigation of the mechanism of domain closure in citrate synthase by molecular dynamics simulation 1 Edited by R. Huber. <i>Journal of Molecular Biology</i> , 2001, 310, 1039-1053.	4.2	45
33	Selective Excitation of Native Fluctuations during Thermal Unfolding Simulations: Horse Heart Cytochrome c as a Case Study. <i>Biophysical Journal</i> , 2003, 84, 1876-1883.	0.5	45
34	Understanding a Mechanism of Organic Cosolvent Inactivation in Heme Monooxygenase P450 BM-3. <i>Journal of the American Chemical Society</i> , 2007, 129, 5786-5787.	13.7	44
35	Molecular Dynamics Simulations of Lignin Peroxidase in Solution. <i>Biophysical Journal</i> , 2003, 84, 3883-3893.	0.5	40
36	Micellar drug nanocarriers and biomembranes: how do they interact?. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5093.	2.8	40

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37	Transversion-enriched sequence saturation mutagenesis (SeSaM ⁺): A random mutagenesis method with consecutive nucleotide exchanges that complements the bias of error-prone PCR. <i>Biotechnology Journal</i> , 2008, 3, 74-82.	3.5	39
38	Structure and dynamics of 1,2-dimethoxyethane and 1,2-dimethoxypropane in aqueous and non-aqueous solutions: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2011, 135, 164501.	3.0	39
39	Investigating the Accessibility of the Closed Domain Conformation of Citrate Synthase using Essential Dynamics Sampling. <i>Journal of Molecular Biology</i> , 2004, 339, 515-525.	4.2	35
40	Directed Evolution of an Antitumor Drug (Arginine Deiminase PpADI) for Increased Activity at Physiological pH. <i>ChemBioChem</i> , 2010, 11, 691-697.	2.6	35
41	Computer Simulations Study of Biomolecules in Non-Aqueous or Cosolvent/Water Mixture Solutions. <i>Current Protein and Peptide Science</i> , 2008, 9, 407-426.	1.4	34
42	Molecular Dynamics Simulation Study of Chlorophyll a in Different Organic Solvents. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1131-1140.	5.3	34
43	Validation of a hybrid MD-SCF coarse-grained model for DPPC in non-lamellar phases. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	34
44	Interplay between hydrophobic cluster and loop propensity in beta-hairpin formation: A mechanistic study. <i>Protein Science</i> , 2003, 12, 538-550.	7.6	32
45	Challenges of the genetic code for exploring sequence space in directed protein evolution. <i>Biocatalysis and Biotransformation</i> , 2007, 25, 229-241.	2.0	28
46	SeSaM ⁺ Generates a Protein Sequence Space that is Unobtainable by epPCR. <i>ChemBioChem</i> , 2011, 12, 1595-1601.	2.6	28
47	Iterative key-residues interrogation of a phytase with thermostability increasing substitutions identified in directed evolution. <i>Applied Microbiology and Biotechnology</i> , 2016, 100, 227-242.	3.6	28
48	Dynamical Aspects of TEM-1 β -Lactamase Probed by Molecular Dynamics. <i>Journal of Computer-Aided Molecular Design</i> , 2005, 19, 329-340.	2.9	27
49	Synthetic Polymers and Biomembranes. How Do They Interact?: Atomistic Molecular Dynamics Simulation Study of PEO in Contact with a DMPC Lipid Bilayer. <i>Journal of Physical Chemistry B</i> , 2006, 110, 26170-26179.	2.6	27
50	A Potential Antitumor Drug (Arginine Deiminase) Reengineered for Efficient Operation under Physiological Conditions. <i>ChemBioChem</i> , 2010, 11, 2294-2301.	2.6	27
51	Toward understanding the inactivation mechanism of monooxygenase P450 BM-3 by organic cosolvents: A molecular dynamics simulation study. <i>Biopolymers</i> , 2006, 83, 467-476.	2.4	26
52	Structure, dynamics, and function of the monooxygenase P450 BM-3: insights from computer simulations studies. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 273102.	1.8	26
53	Temperature effects on structure and dynamics of the psychrophilic protease subtilisin S41 and its thermostable mutants in solution. <i>Protein Engineering, Design and Selection</i> , 2011, 24, 533-544.	2.1	25
54	Diffusion of 1,2-Dimethoxyethane and 1,2-Dimethoxypropane through Phosphatidycholine Bilayers: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5141-5151.	2.6	24

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55	Structural and dynamic properties of cytochrome P450 BM-3 in pure water and in a dimethylsulfoxide/water mixture. <i>Biopolymers</i> , 2005, 78, 259-267.	2.4	23
56	Temperature Dependence of Looping Rates in a Short Peptide. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2639-2646.	2.6	23
57	The role of active-site Phe87 in modulating the organic co-solvent tolerance of cytochrome P450 BM3 monooxygenase. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2012, 68, 1013-1017.	0.7	23
58	Spontaneous insertion of carbon nanotube bundles inside biomembranes: A hybrid particle-field coarse-grained molecular dynamics study. <i>Chemical Physics Letters</i> , 2014, 595-596, 156-166.	2.6	23
59	Molecular Dynamics Simulation of Water Near Nanostructured Hydrophobic Surfaces: Interfacial Energies. <i>ChemPhysChem</i> , 2005, 6, 1641-1649.	2.1	21
60	Are transversion mutations better? A Mutagenesis Assistant Program analysis on P450 BM-3 heme domain. <i>Biotechnology Journal</i> , 2007, 2, 133-142.	3.5	21
61	Directed Evolution of Subtilisin E into a Highly Active and Guanidinium Chloride- and Sodium Dodecylsulfate-tolerant Protease. <i>ChemBioChem</i> , 2012, 13, 691-699.	2.6	21
62	P450 BM3 crystal structures reveal the role of the charged surface residue Lys/Arg184 in inversion of enantioselective styrene epoxidation. <i>Chemical Communications</i> , 2013, 49, 4694.	4.1	21
63	Insight into the redox partner interaction mechanism in cytochrome P450BM3 using molecular dynamics simulations. <i>Biopolymers</i> , 2014, 101, 197-209.	2.4	21
64	MAP ^{2.0} 3D: A Sequence/Structure Based Server for Protein Engineering. <i>ACS Synthetic Biology</i> , 2012, 1, 139-150.	3.8	19
65	Application of the quasi-Gaussian entropy theory to molecular dynamics simulations of Lennard-Jones fluids. <i>Journal of Chemical Physics</i> , 1998, 109, 6358-6363.	3.0	18
66	Structural and Dynamic Properties of the CAGQW Peptide in Water: A Molecular Dynamics Simulation Study Using Different Force Fields. <i>Journal of Physical Chemistry B</i> , 2004, 108, 18734-18742.	2.6	16
67	A computational protocol to predict suitable redox mediators for substitution of NAD(P)H in P450 monooxygenases. <i>Journal of Molecular Catalysis B: Enzymatic</i> , 2013, 88, 47-51.	1.8	16
68	Conformational dynamics of active site loop in <i>Escherichia coli</i> phytase. <i>Biopolymers</i> , 2010, 93, 994-1002.	2.4	15
69	Theoretical Study of Binding and Permeation of Ether-Based Polymers through Interfaces. <i>Journal of Physical Chemistry B</i> , 2013, 117, 14723-14731.	2.6	14
70	Coating Mechanisms of Single-Walled Carbon Nanotube by Linear Polyether Surfactants: Insights from Computer Simulations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 18069-18078.	3.1	14
71	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. <i>Journal of Computer-Aided Molecular Design</i> , 2002, 16, 213-225.	2.9	13
72	Conformational Dynamics of the FMN-Binding Reductase Domain of Monooxygenase P450BM-3. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 96-105.	5.3	12

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73	Insights on activity and stability of subtilisin E towards guanidinium chloride and sodium dodecylsulfate. <i>Journal of Biotechnology</i> , 2014, 169, 87-94.	3.8	12
74	Strings-to-Rings Transition and Antiparallel Dipole Alignment in Two-Dimensional Methanols. <i>Nano Letters</i> , 2016, 16, 3142-3147.	9.1	12
75	Adsorption mechanism of an antimicrobial peptide on carbonaceous surfaces: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2017, 146, 074703.	3.0	12
76	The Influence of Trifluoromethyl Groups on the Miscibility of Fluorinated Alcohols with Water: A Molecular Dynamics Simulation Study of 1,1,1-Trifluoropropan-2-ol in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2003, 107, 4855-4861.	2.6	11
77	Prediction of the liquid-vapor equilibrium pressure using the quasi-Gaussian entropy theory. <i>Journal of Chemical Physics</i> , 1996, 105, 7022-7025.	3.0	10
78	Chiral discrimination in liquid 1,1,1-trifluoropropan-2-ol: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2003, 119, 7289-7296.	3.0	9
79	A Theoretical Model for the Folding/Unfolding Thermodynamics of Single-Domain Proteins, Based on the Quasi-Gaussian Entropy Theory. <i>Journal of Physical Chemistry B</i> , 2004, 108, 5756-5762.	2.6	9
80	dRTP and dPTP a complementary nucleotide couple for the Sequence Saturation Mutagenesis (SeSaM) method. <i>Journal of Molecular Catalysis B: Enzymatic</i> , 2012, 84, 40-47.	1.8	9
81	Modelling the adsorption of proteins to nanoparticles at the solid-liquid interface. <i>Journal of Colloid and Interface Science</i> , 2022, 605, 286-295.	9.4	9
82	Molecular dynamics simulation of the interaction between the complex iron-sulfur flavoprotein glutamate synthase and its substrates. <i>Protein Science</i> , 2008, 13, 2979-2991.	7.6	8
83	Study of structural and dynamic properties of liquid phenyltrimethoxysilane. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11864.	2.8	7
84	Cosolvent, ions, and temperature effects on the structural properties of cecropin A-Magainin 2 hybrid peptide in solutions. <i>Biopolymers</i> , 2015, 103, 1-14.	2.4	7
85	Molecular Properties of Astaxanthin in Water/Ethanol Solutions from Computer Simulations. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9322-9328.	2.6	7
86	Conformational and Electronic Properties of a Microperoxidase in Aqueous Solution: A Computational Study. <i>ChemPhysChem</i> , 2005, 6, 681-689.	2.1	6
87	Unraveling Binding Effects of Cobalt(II) Sepulchrate with the Monooxygenase P450 BM-3 Heme Domain Using Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 353-363.	5.3	6
88	A Short Introduction to the Molecular Dynamics Simulation of Nanomaterials. , 2018, , 123-155.		6
89	The Mutagenesis Assistant Program. <i>Methods in Molecular Biology</i> , 2014, 1179, 279-290.	0.9	5
90	Development of a parallel molecular dynamics code on SIMD computers: Algorithm for use of pair list criterion. <i>Journal of Computational Chemistry</i> , 1998, 19, 685-694.	3.3	4

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91	Characterization of liquid behaviour by means of local density fluctuations. Journal of Molecular Liquids, 2005, 117, 17-21.	4.9	2
92	Theoretical Study of Nanostructured Biopolymers Using Molecular Dynamics Simulations: A Practical Introduction. Nanoscience and Technology, 2007, , 555-585.	1.5	2
93	Free Energy Profile of Domain Movement in Ligand-Free Citrate Synthase. Journal of Physical Chemistry B, 2019, 123, 1998-2004.	2.6	1
94	The Molecular Dynamics Simulation of Peptides on Gold Nanosurfaces. Methods in Molecular Biology, 2020, 2118, 177-197.	0.9	1
95	Inside Cover: A Potential Antitumor Drug (Arginine Deiminase) Reengineered for Efficient Operation under Physiological Conditions (ChemBioChem 16/2010). ChemBioChem, 2010, 11, 2194-2194.	2.6	0
96	Validation of a hybrid MD-SCF coarse-grained model for DPPC in non-lamellar phases. Highlights in Theoretical Chemistry, 2013, , 169-184.	0.0	0