Danilo Roccatano

List of Publications by Year
in descending order

96 papers	3,997 citations	108046 37 h-index	150775 59 g-index
98 all docs	98 docs citations	98 times ranked	5256 citing authors

#	Article	IF	Citations
1	Modelling the adsorption of proteins to nanoparticles at the solid-liquid interface. Journal of Colloid and Interface Science, 2022, 605, 286-295.	5.0	9
2	The Molecular Dynamics Simulation of Peptides on Gold Nanosurfaces. Methods in Molecular Biology, 2020, 2118, 177-197.	0.4	1
3	Free Energy Profile of Domain Movement in Ligand-Free Citrate Synthase. Journal of Physical Chemistry B, 2019, 123, 1998-2004.	1.2	1
4	Modular assembly of proteins on nanoparticles. Nature Communications, 2018, 9, 1489.	5.8	76
5	A Short Introduction to the Molecular Dynamics Simulation of Nanomaterials. , 2018, , 123-155.		6
6	Adsorption mechanism of an antimicrobial peptide on carbonaceous surfaces: A molecular dynamics study. Journal of Chemical Physics, 2017, 146, 074703.	1.2	12
7	Molecular Properties of Astaxanthin in Water/Ethanol Solutions from Computer Simulations. Journal of Physical Chemistry B, 2016, 120, 9322-9328.	1.2	7
8	Strings-to-Rings Transition and Antiparallel Dipole Alignment in Two-Dimensional Methanols. Nano Letters, 2016, 16, 3142-3147.	4.5	12
9	Unraveling Binding Effects of Cobalt(II) Sepulchrate with the Monooxygenase P450 BM-3 Heme Domain Using Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2016, 12, 353-363.	2.3	6
10	Iterative key-residues interrogation of a phytase with thermostability increasing substitutions identified in directed evolution. Applied Microbiology and Biotechnology, 2016, 100, 227-242.	1.7	28
11	Cosolvent, ions, and temperature effects on the structural properties of cecropin Aâ€Magainin 2 hybrid peptide in solutions. Biopolymers, 2015, 103, 1-14.	1.2	7
12	Structure, dynamics, and function of the monooxygenase P450 BM-3: insights from computer simulations studies. Journal of Physics Condensed Matter, 2015, 27, 273102.	0.7	26
13	Insight into the redox partner interaction mechanism in cytochrome P450BMâ€ƀ using molecular dynamics simulations. Biopolymers, 2014, 101, 197-209.	1.2	21
14	Insights on activity and stability of subtilisin E towards guanidinium chloride and sodium dodecylsulfate. Journal of Biotechnology, 2014, 169, 87-94.	1.9	12
15	Micellar drug nanocarriers and biomembranes: how do they interact?. Physical Chemistry Chemical Physics, 2014, 16, 5093.	1.3	40
16	Coating Mechanisms of Single-Walled Carbon Nanotube by Linear Polyether Surfactants: Insights from Computer Simulations. Journal of Physical Chemistry C, 2014, 118, 18069-18078.	1.5	14
17	Spontaneous insertion of carbon nanotube bundles inside biomembranes: A hybrid particle-field coarse-grained molecular dynamics study. Chemical Physics Letters, 2014, 595-596, 156-166.	1.2	23
18	The Mutagenesis Assistant Program. Methods in Molecular Biology, 2014, 1179, 279-290.	0.4	5

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19	P450 BM3 crystal structures reveal the role of the charged surface residue Lys/Arg184 in inversion of enantioselective styrene epoxidation. Chemical Communications, 2013, 49, 4694.	2.2	21
20	A computational protocol to predict suitable redox mediators for substitution of NAD(P)H in P450 monooxygenases. Journal of Molecular Catalysis B: Enzymatic, 2013, 88, 47-51.	1.8	16
21	Interaction of Curcumin with PEOâ€“PPOâ€“PEO Block Copolymers: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2013, 117, 3250-3257.	1.2	50
22	Conformational Dynamics of the FMN-Binding Reductase Domain of Monooxygenase P450BM-3. Journal of Chemical Theory and Computation, 2013, 9, 96-105.	2.3	12
23	Theoretical Study of Binding and Permeation of Ether-Based Polymers through Interfaces. Journal of Physical Chemistry B, 2013, 117, 14723-14731.	1.2	14
24	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
25	The role of active-site Phe87 in modulating the organic co-solvent tolerance of cytochrome P450 BM3 monooxygenase. Acta Crystallographica Section F: Structural Biology Communications, 2012, 68, 1013-1017.	0.7	23
26	Diffusion of 1,2-Dimethoxyethane and 1,2-Dimethoxypropane through Phosphatidycholine Bilayers: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2012, 116, 5141-5151.	1.2	24
27	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.	1.2	77
28	COMPUTER-AIDED PROTEIN DIRECTED EVOLUTION: A REVIEW OF WEB SERVERS, DATABASES AND OTHER COMPUTATIONAL TOOLS FOR PROTEIN ENGINEERING. Computational and Structural Biotechnology Journal, 2012, 2, e201209008.	1.9	52
29	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. Journal of Chemical Physics, 2012, 136, 124901.	1.2	59
30	MAP^{2.0}3D: A Sequence/Structure Based Server for Protein Engineering. ACS Synthetic Biology, 2012, 1, 139-150.	1.9	19
31	dRTP and dPTP a complementary nucleotide couple for the Sequence Saturation Mutagenesis (SeSaM) method. Journal of Molecular Catalysis B: Enzymatic, 2012, 84, 40-47.	1.8	9
32	Structure and Dynamics of Dodecaborate Clusters in Water. Inorganic Chemistry, 2012, 51, 4894-4896.	1.9	47
33	Directed Evolution of Subtilisin E into a Highly Active and Guanidinium Chlorideâ€•and Sodium Dodecylsulfateâ€Tolerant Protease. ChemBioChem, 2012, 13, 691-699.	1.3	21
34	Validation of a hybrid MD-SCF coarse-grained model for DPPC in non-lamellar phases. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	34
35	Directed evolution of a highly active Yersinia mollaretii phytase. Applied Microbiology and Biotechnology, 2012, 95, 405-418.	1.7	64
36	Study of structural and dynamic properties of liquid phenyltrimethoxysilane. Physical Chemistry Chemical Physics, 2011, 13, 11864.	1.3	7

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37	Structure and dynamics of 1,2-dimethoxyethane and 1,2-dimethoxypropane in aqueous and non-aqueous solutions: A molecular dynamics study. Journal of Chemical Physics, 2011, 135, 164501.	1.2	39
38	Molecular Dynamics Simulation Study of Chlorophyll a in Different Organic Solvents. Journal of Chemical Theory and Computation, 2011, 7, 1131-1140.	2.3	34
39	Hybrid Particle-Field Coarse-Grained Models for Biological Phospholipids. Journal of Chemical Theory and Computation, 2011, 7, 2947-2962.	2.3	58
40	SeSaMâ€Tvâ€I Generates a Protein Sequence Space that is Unobtainable by epPCR. ChemBioChem, 2011, 12, 1595-1601.	1.3	28
41	Temperature effects on structure and dynamics of the psychrophilic protease subtilisin S41 and its thermostable mutants in solution. Protein Engineering, Design and Selection, 2011, 24, 533-544.	1.0	25
42	Directed Evolution of an Antitumor Drug (Arginine Deiminase PpADI) for Increased Activity at Physiological pH. ChemBioChem, 2010, 11, 691-697.	1.3	35
43	A Potential Antitumor Drug (Arginine Deiminase) Reengineered for Efficient Operation under Physiological Conditions. ChemBioChem, 2010, 11, 2294-2301.	1.3	27
44	Inside Cover: A Potential Antitumor Drug (Arginine Deiminase) Reengineered for Efficient Operation under Physiological Conditions (ChemBioChem 16/2010). ChemBioChem, 2010, 11, 2194-2194.	1.3	0
45	Conformational dynamics of active site loop in Escherichia coli phytase. Biopolymers, 2010, 93, 994-1002.	1.2	15
46	Functionalized Nanocompartments (Synthosomes) with a Reductionâ€Triggered Release System. Angewandte Chemie - International Edition, 2008, 47, 7029-7031.	7.2	63
47	Transversionâ€enriched sequence saturation mutagenesis (SeSaMâ€Tv⁺): A random mutagenesis method with consecutive nucleotide exchanges that complements the bias of errorâ€prone PCR. Biotechnology Journal, 2008, 3, 74-82.	1.8	39
48	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
49	Ionic liquid effects on the activity of monooxygenase P450 BM-3. Green Chemistry, 2008, 10, 117-123.	4.6	46
50	Computer Simulations Study of Biomolecules in Non-Aqueous or Cosolvent/Water Mixture Solutions. Current Protein and Peptide Science, 2008, 9, 407-426.	0.7	34
51	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.	1.0	68
52	Challenges of the genetic code for exploring sequence space in directed protein evolution. Biocatalysis and Biotransformation, 2007, 25, 229-241.	1.1	28
53	A 10-Ã... Spectroscopic Ruler Applied to Short Polyprolines. Journal of the American Chemical Society, 2007, 129, 9762-9772.	6.6	87
54	Temperature Dependence of Looping Rates in a Short Peptide. Journal of Physical Chemistry B, 2007, 111, 2639-2646.	1.2	23

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55	Understanding a Mechanism of Organic Cosolvent Inactivation in Heme Monooxygenase P450 BM-3. Journal of the American Chemical Society, 2007, 129, 5786-5787.	6.6	44
56	Structural flexibility of the nucleosome core particle at atomic resolution studied by molecular dynamics simulation. Biopolymers, 2007, 85, 407-421.	1.2	86
57	Steering directed protein evolution: strategies to manage combinatorial complexity of mutant libraries. Environmental Microbiology, 2007, 9, 2645-2659.	1.8	59
58	Are transversion mutations better? A Mutagenesis Assistant Program analysis on P450 BM-3 heme domain. Biotechnology Journal, 2007, 2, 133-142.	1.8	21
59	Theoretical Study of Nanostructured Biopolymers Using Molecular Dynamics Simulations: A Practical Introduction. Nanoscience and Technology, 2007, , 555-585.	1.5	2
60	Distance Distributions of Short Polypeptides Recovered by Fluorescence Resonance Energy Transfer in the 10 Ã... Domain. Journal of the American Chemical Society, 2006, 128, 8118-8119.	6.6	68
61	Synthetic Polymers and Biomembranes. How Do They Interact?:Â Atomistic Molecular Dynamics Simulation Study of PEO in Contact with a DMPC Lipid Bilayer. Journal of Physical Chemistry B, 2006, 110, 26170-26179.	1.2	27
62	A Statistical Analysis of Random Mutagenesis Methods Used for Directed Protein Evolution. Journal of Molecular Biology, 2006, 355, 858-871.	2.0	132
63	Toward understanding the inactivation mechanism of monooxygenase P450 BM-3 by organic cosolvents: A molecular dynamics simulation study. Biopolymers, 2006, 83, 467-476.	1.2	26
64	Effect of hexafluoroisopropanol alcohol on the structure of melittin: A molecular dynamics simulation study. Protein Science, 2005, 14, 2582-2589.	3.1	76
65	Conformational and Electronic Properties of a Microperoxidase in Aqueous Solution: A Computational Study. ChemPhysChem, 2005, 6, 681-689.	1.0	6
66	Molecular Dynamics Simulation of Water Near Nanostructured Hydrophobic Surfaces: Interfacial Energies. ChemPhysChem, 2005, 6, 1641-1649.	1.0	21
67	Structural and dynamic properties of cytochrome P450 BM-3 in pure water and in a dimethylsulfoxide/water mixture. Biopolymers, 2005, 78, 259-267.	1.2	23
68	Dynamical Aspects of TEM-1 Î²-Lactamase Probed by Molecular Dynamics. Journal of Computer-Aided Molecular Design, 2005, 19, 329-340.	1.3	27
69	Characterization of liquid behaviour by means of local density fluctuations. Journal of Molecular Liquids, 2005, 117, 17-21.	2.3	2
70	Sensitive Assay for Laboratory Evolution of Hydroxylases toward Aromatic and Heterocyclic Compounds. Journal of Biomolecular Screening, 2005, 10, 246-252.	2.6	46
71	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
72	Structural and Dynamic Properties of the CAGQW Peptide in Water:â€‰ A Molecular Dynamics Simulation Study Using Different Force Fields. Journal of Physical Chemistry B, 2004, 108, 18734-18742.	1.2	16

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73	A Theoretical Model for the Folding/Unfolding Thermodynamics of Single-Domain Proteins, Based on the Quasi-Gaussian Entropy Theory. Journal of Physical Chemistry B, 2004, 108, 5756-5762.	1.2	9
74	Extended Molecular Dynamics Simulation of the Carbon Monoxide Migration in Sperm Whale Myoglobin. Biophysical Journal, 2004, 86, 3855-3862.	0.2	129
75	Investigating the Accessibility of the Closed Domain Conformation of Citrate Synthase using Essential Dynamics Sampling. Journal of Molecular Biology, 2004, 339, 515-525.	2.0	35
76	Interplay between hydrophobic cluster and loop propensity in beta-hairpin formation: A mechanistic study. Protein Science, 2003, 12, 538-550.	3.1	32
77	The Influence of Trifluoromethyl Groups on the Miscibility of Fluorinated Alcohols with Water:Â A Molecular Dynamics Simulation Study of 1,1,1-Trifluoropropan-2-ol in Aqueous Solution. Journal of Physical Chemistry B, 2003, 107, 4855-4861.	1.2	11
78	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
79	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
80	Molecular Dynamics Simulations of Lignin Peroxidase in Solution. Biophysical Journal, 2003, 84, 3883-3893.	0.2	40
81	Chiral discrimination in liquid 1,1,1-trifluoropropan-2-ol: A molecular dynamics study. Journal of Chemical Physics, 2003, 119, 7289-7296.	1.2	9
82	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.	3.3	465
83	Folding and stability of the three-stranded ?-sheet peptide Betanova: Insights from molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2002, 46, 380-392.	1.5	50
84	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
85	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.	1.2	72
86	Investigation of the mechanism of domain closure in citrate synthase by molecular dynamics simulation 1 1Edited by R. Huber. Journal of Molecular Biology, 2001, 310, 1039-1053.	2.0	45
87	A New 2,2,2-Trifluoroethanol Model for Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2000, 104, 12347-12354.	1.2	106
88	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
89	Docking of flexible ligands to flexible receptors in solution by molecular dynamics simulation. , 1999, 35, 153-162.		118
90	Development of a parallel molecular dynamics code on SIMD computers: Algorithm for use of pair list criterion. Journal of Computational Chemistry, 1998, 19, 685-694.	1.5	4

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91	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 Sr2+ in methanol solution. Journal of Chemical Physics, 1998, 108, 9487-9497.	1.2	45
92	Application of the quasi-Gaussian entropy theory to molecular dynamics simulations of Lennard-Jones fluids. Journal of Chemical Physics, 1998, 109, 6358-6363.	1.2	18
93	Multielectron excitations at theLedges of barium in aqueous solution. Physical Review B, 1996, 54, 12129-12138.	1.1	48
94	Prediction of the liquidâ€“vapor equilibrium pressure using the quasiâ€Gaussian entropy theory. Journal of Chemical Physics, 1996, 105, 7022-7025.	1.2	10
95	Molecular dynamics simulation of the docking of substrates to proteins. Proteins: Structure, Function and Bioinformatics, 1994, 19, 174-182.	1.5	96
96	An extended xâ€ray absorption fine structure study of aqueous solutions by employing molecular dynamics simulations. Journal of Chemical Physics, 1994, 100, 985-994.	1.2	133