Piero Procacci

List of Publications by Year
in descending order

123	4,138	109137	133063
papers	citations	35 h-index	59 g-index

128	128	128	3716
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Stacking and T-shape Competition in Aromaticâ^'Aromatic Amino Acid Interactions. Journal of the American Chemical Society, 2002, 124, 6133-6143.	6.6	233
2	ORAC: A Molecular dynamics program to simulate complex molecular systems with realistic electrostatic interactions. Journal of Computational Chemistry, 1997, 18, 1848-1862.	1.5	163
3	Identification of potential binders of the main protease 3CLpro of the COVID-19 via structure-based ligand design and molecular modeling. Chemical Physics Letters, 2020, 750, 137489.	1.2	133
4	Assessment of GAFF2 and OPLS-AA General Force Fields in Combination with the Water Models TIP3P, SPCE, and OPC3 for the Solvation Free Energy of Druglike Organic Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1983-1995.	2.3	131
5	Glycerol condensed phases Part II.A molecular dynamics study of the conformational structure and hydrogen bonding. Physical Chemistry Chemical Physics, 1999, 1, 879-885.	1.3	126
6	A transferable polarizable electrostatic force field for molecular mechanics based on the chemical potential equalization principle. Journal of Chemical Physics, 2002, 117, 9175-9189.	1.2	124
7	Electrical response in chemical potential equalization schemes. Journal of Chemical Physics, 1999, 111, 8569-8575.	1.2	115
8	Self-healing Umbrella Sampling:Â A Non-equilibrium Approach for Quantitative Free Energy Calculations. Journal of Physical Chemistry B, 2006, 110, 14011-14013.	1.2	114
9	Glycerol condensed phases Part I. A molecular dynamics study. Physical Chemistry Chemical Physics, 1999, 1, 871-877.	1.3	112
10	Metadynamics Simulation of Prion Protein:Â Î²-Structure Stability and the Early Stages of Misfolding. Journal of the American Chemical Society, 2006, 128, 2705-2710.	6.6	105
11	Coordinates scaling and multiple time step algorithms for simulation of solvated proteins in the NPT ensemble. Journal of Chemical Physics, 1998, 109, 5194-5202.	1.2	97
12	A Very Fast Molecular Dynamics Method To Simulate Biomolecular Systems with Realistic Electrostatic Interactions. The Journal of Physical Chemistry, 1996, 100, 10464-10468.	2.9	88
13	Anab initio force field for the cofactors of bacterial photosynthesis. Journal of Computational Chemistry, 2003, 24, 129-142.	1.5	79
14	Thermodynamics of stacking interactions in proteins. Physical Chemistry Chemical Physics, 2008, 10, 2673.	1.3	79
15	Title is missing!. Journal of Computational Chemistry, 1997, 18, 1848.	1.5	77
16	Key Role of the Polarization Anisotropy of Water in Modeling Classical Polarizable Force Fields. Journal of Physical Chemistry A, 2007, 111, 8170-8176.	1.1	76
17	The nature of intermolecular interactions between aromatic amino acid residues. Proteins: Structure, Function and Bioinformatics, 2002, 48, 117-125.	1.5	72
18	Taming the Ewald sum in molecular dynamics simulations of solvated proteins via a multiple time step algorithm. Journal of Chemical Physics, 1996, 104, 3003-3012.	1.2	71

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19	ORAC: A molecular dynamics simulation program to explore free energy surfaces in biomolecular systems at the atomistic level. Journal of Computational Chemistry, 2010, 31, 1106-1116.	1.5	67
20	Calculation of optical spectra in liquid methanol using molecular dynamics and the chemical potential equalization method. Journal of Chemical Physics, 1999, 111, 4218-4229.	1.2	66
21	Simulated structure, dynamics, and vibrational spectra of liquid benzene. Journal of Chemical Physics, 2000, 113, 6851-6863.	1.2	65
22	Density Functional Calculation of Structural and Vibrational Properties of Glycerol. Journal of Physical Chemistry A, 2000, 104, 5351-5357.	1.1	62
23	Electrostatic calculations and multiple time scales in molecular dynamics simulation of flexible molecular systems. Journal of Chemical Physics, 1998, 108, 8799-8803.	1.2	60
24	Crooks equation for steered molecular dynamics using a NosÃ©-Hoover thermostat. Journal of Chemical Physics, 2006, 125, 164101.	1.2	60
25	Misfolding Pathways of the Prion Protein Probed by Molecular Dynamics Simulations. Biophysical Journal, 2005, 88, 1334-1343.	0.2	58
26	Computer simulation of solid C60 using multiple timeâ€step algorithms. Journal of Chemical Physics, 1994, 101, 2421-2431.	1.2	47
27	Multiple time scale methods for constant pressure molecular dynamics simulations of molecular systems. Molecular Physics, 1994, 83, 255-272.	0.8	46
28	Upgrading and Validation of the AMBER Force Field for Histidine and Cysteine Zinc(II)-Binding Residues in Sites with Four Protein Ligands. Journal of Chemical Information and Modeling, 2019, 59, 3803-3816.	2.5	42
29	Interaction between Aromatic Residues. Molecular Dynamics and ab Initio Exploration of the Potential Energy Surface of the Tryptophanâ^'Histidine Pair. Journal of Physical Chemistry B, 2000, 104, 1108-1114.	1.2	41
30	Hybrid MPI/OpenMP Implementation of the ORAC Molecular Dynamics Program for Generalized Ensemble and Fast Switching Alchemical Simulations. Journal of Chemical Information and Modeling, 2016, 56, 1117-1121.	2.5	41
31	Is the T-Shaped Toluene Dimer a Stable Intermolecular Complex?. Journal of Physical Chemistry A, 2002, 106, 2945-2948.	1.1	40
32	Polarization response of water and methanol investigated by a polarizable force field and density functional theory calculations: Implications for charge transfer. Journal of Chemical Physics, 2005, 122, 074504.	1.2	40
33	PrimaDORAC: A Free Web Interface for the Assignment of Partial Charges, Chemical Topology, and Bonded Parameters in Organic or Drug Molecules. Journal of Chemical Information and Modeling, 2017, 57, 1240-1245.	2.5	39
34	Statistical Mechanics of Ligandâ€“Receptor Noncovalent Association, Revisited: Binding Site and Standard State Volumes in Modern Alchemical Theories. Journal of Chemical Theory and Computation, 2017, 13, 1924-1933.	2.3	39
35	Generalization of the Jarzynski and Crooks nonequilibrium work theorems in molecular dynamics simulations. Physical Review E, 2007, 75, 050101.	0.8	37
36	A potential of mean force estimator based on nonequilibrium work exponential averages. Physical Chemistry Chemical Physics, 2009, 11, 1152.	1.3	37

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37	Fast Switching Alchemical Transformations in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 2813-2823.	2.3	36
38	Comparing polarizable force fields to ab initio calculations reveals nonclassical effects in condensed phases. Journal of Chemical Physics, 2005, 122, 234107.	1.2	34
39	Efficient Nonequilibrium Method for Binding Free Energy Calculations in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 423-435.	2.3	34
40	II. Dissociation free energies in drugâ€“receptor systems via nonequilibrium alchemical simulations: application to the FK506-related immunophilin ligands. Physical Chemistry Chemical Physics, 2016, 18, 15005-15018.	1.3	34
41	Characterization of the non-covalent interaction between the PF-07321332 inhibitor and the SARS-CoV-2 main protease. Journal of Molecular Graphics and Modelling, 2022, 110, 108042.	1.3	34
42	A general algorithm for computing Voronoi volumes: Application to the hydrated crystal of myoglobin. International Journal of Quantum Chemistry, 1992, 42, 1515-1528.	1.0	33
43	Calculation of the potential of mean force from nonequilibrium measurements via maximum likelihood estimators. Physical Review E, 2008, 77, 031104.	0.8	33
44	Vibrational frequencies of C70. Chemical Physics Letters, 1992, 195, 347-351.	1.2	32
45	Conformational Distribution of Gas-phase Glycerol. Journal of Physical Chemistry A, 2000, 104, 11220-11222.	1.1	32
46	Anharmonic calculation of bandwidths and frequency shifts in crystalline CO2. Chemical Physics, 1987, 116, 171-186.	0.9	31
47	Determination of the Potential of Mean Force of Aromatic Amino Acid Complexes in Various Solvents Using Molecular Dynamics Simulations:Â The Case of the Tryptophanâ^'Histidine Pair. Journal of Physical Chemistry B, 2001, 105, 7835-7846.	1.2	29
48	SAMPL6 hostâ€“guest blind predictions using a non equilibrium alchemical approach. Journal of Computer-Aided Molecular Design, 2018, 32, 965-982.	1.3	29
49	The Precise Chemicalâ€“Physical Nature of the Pharmacore in FK506 Binding Protein Inhibition: ElteX, a New Class of Nanomolar FKBP12 Ligands. Journal of Medicinal Chemistry, 2013, 56, 1041-1051.	2.9	28
50	I. Dissociation free energies of drugâ€“receptor systems via non-equilibrium alchemical simulations: a theoretical framework. Physical Chemistry Chemical Physics, 2016, 18, 14991-15004.	1.3	28
51	Virtual Double-System Single-Box: A Nonequilibrium Alchemical Technique for Absolute Binding Free Energy Calculations: Application to Ligands of the SARS-CoV-2 Main Protease. Journal of Chemical Theory and Computation, 2020, 16, 7160-7172.	2.3	27
52	Upgraded AMBER Force Field for Zinc-Binding Residues and Ligands for Predicting Structural Properties and Binding Affinities in Zinc-Proteins. ACS Omega, 2020, 5, 15301-15310.	1.6	27
53	Mycotoxins aptasensing: From molecular docking to electrochemical detection of deoxynivalenol. Bioelectrochemistry, 2021, 138, 107691.	2.4	27
54	Vibrational properties of Xeâ€”fullerene adducts. A molecular dynamics approach. Chemical Physics Letters, 1992, 200, 39-45.	1.2	24

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55	The far-infrared spectrum of crystalline fullerene C60. The Journal of Physical Chemistry, 1993, 97, 10580-10584.	2.9	22
56	Unbiased free energy estimates in fast nonequilibrium transformations using Gaussian mixtures. Journal of Chemical Physics, 2015, 142, 154117.	1.2	22
57	Interaction of hydroxychloroquine with SARS-CoV2 functional proteins using all-atoms non-equilibrium alchemical simulations. Chemical Communications, 2020, 56, 8854-8856.	2.2	22
58	Hummer and Szabo-like Potential of Mean Force Estimator for Bidirectional Nonequilibrium Pulling Experiments/Simulations. Journal of Physical Chemistry B, 2010, 114, 9546-9554.	1.2	20
59	Alchemical determination of drug-receptor binding free energy: Where we stand and where we could move to. Journal of Molecular Graphics and Modelling, 2017, 71, 233-241.	1.3	20
60	Regioselective Electrophilic Access to Naphtho[1,2-b:8,7-bâ€²]- and -[1,2-b:5,6-bâ€²]dithiophenes. Journal of Organic Chemistry, 2013, 78, 3496-3502.	1.7	19
61	Methodological uncertainties in drug-receptor binding free energy predictions based on classical molecular dynamics. Current Opinion in Structural Biology, 2021, 67, 127-134.	2.6	19
62	Solvation free energies via alchemical simulations: let's get honest about sampling, once more. Physical Chemistry Chemical Physics, 2019, 21, 13826-13834.	1.3	18
63	Anharmonic lattice dynamics and computer simulation for simple model systems. Physical Review B, 1992, 45, 2113-2125.	1.1	17
64	Molecular dynamics of glass-forming liquids: Structure and dynamics of liquid metatoluidine. Journal of Chemical Physics, 2002, 116, 6205-6215.	1.2	17
65	Towards a polarizable force field for molecular liquids. Journal of Molecular Liquids, 2002, 96-97, 87-100.	2.3	17
66	Multiple Bennett acceptance ratio made easy for replica exchange simulations. Journal of Chemical Physics, 2013, 139, 124105.	1.2	17
67	New Perspective on How and Why Immunophilin FK506-Related Ligands Work. Journal of Physical Chemistry Letters, 2011, 2, 2834-2839.	2.1	16
68	SAMPL7 blind predictions using nonequilibrium alchemical approaches. Journal of Computer-Aided Molecular Design, 2021, 35, 37-47.	1.3	16
69	Inter-residue and solvent-residue interactions in proteins: A statistical study on experimental structures. Proteins: Structure, Function and Bioinformatics, 2004, 55, 139-151.	1.5	15
70	Numerical verification of the generalized Crooks nonequilibrium work theorem for non-Hamiltonian molecular dynamics simulations. Journal of Chemical Physics, 2007, 127, 034110.	1.2	15
71	Energy dissipation asymmetry in the non equilibrium folding/unfolding of the single molecule alanine decapeptide. Chemical Physics, 2010, 375, 8-15.	0.9	15
72	Molecular dynamics and anharmonic effects in the phonon spectra of solid carbon dioxide. Chemical Physics, 1987, 117, 355-366.	0.9	14

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73	Behavior of polarizable models in presence of strong electric fields. I. Origin of nonlinear effects in water point-charge systems. Journal of Chemical Physics, 2005, 123, 194109.	1.2	14
74	Recovering the Crooks equation for dynamical systems in the isothermal-isobaric ensemble: A strategy based on the equations of motion. Journal of Chemical Physics, 2007, 126, 044502.	1.2	14
75	Binding Free Energies of Hostâ€“Guest Systems by Nonequilibrium Alchemical Simulations with Constrained Dynamics: Theoretical Framework. Journal of Chemical Theory and Computation, 2017, 13, 5874-5886.	2.3	14
76	Binding Free Energies of Hostâ€“Guest Systems by Nonequilibrium Alchemical Simulations with Constrained Dynamics: Illustrative Calculations and Numerical Validation. Journal of Chemical Theory and Computation, 2017, 13, 5887-5899.	2.3	14
77	Equation of motion for the Greenâ€™s function in anharmonic solids. Physical Review B, 1992, 46, 6141-6149.	1.1	13
78	Dynamical and structural correlation in supercooled liquids: A molecular dynamics investigation of m-toluidine. Journal of Chemical Physics, 2003, 119, 357-363.	1.2	13
79	Conformational Landscape of N-Glycosylated Peptides Detecting Autoantibodies in Multiple Sclerosis, Revealed by Hamiltonian Replica Exchange. Journal of Physical Chemistry B, 2012, 116, 5458-5467.	1.2	13
80	Energy-Driven Undocking (EDU-HREM) in Solute Tempering Replica Exchange Simulations. Journal of Chemical Theory and Computation, 2014, 10, 439-450.	2.3	13
81	Myeloid Cell Leukemia 1 Inhibition: An in Silico Study Using Non-equilibrium Fast Double Annihilation Technology. Journal of Chemical Theory and Computation, 2018, 14, 3890-3902.	2.3	13
82	Accuracy, precision, and efficiency of nonequilibrium alchemical methods for computing free energies of solvation. I. Bidirectional approaches. Journal of Chemical Physics, 2019, 151, 144113.	1.2	13
83	Precision and computational efficiency of nonequilibrium alchemical methods for computing free energies of solvation. II. Unidirectional estimates. Journal of Chemical Physics, 2019, 151, 144115.	1.2	12
84	Intraligand Hydrophobic Interactions Rationalize Drug Affinities for Peptidylâ^'Prolyl Cisâ^'Trans Isomerase Protein. Journal of Physical Chemistry B, 2011, 115, 6193-6201.	1.2	11
85	Virtual Double-System Single-Box for Absolute Dissociation Free Energy Calculations in GROMACS. Journal of Chemical Information and Modeling, 2021, 61, 5320-5326.	2.5	11
86	Efficient calculation of high-order self-energy corrections to phonon linewidths: Application to Î±-nitrogen. Physical Review B, 1993, 47, 11124-11133.	1.1	10
87	Energetic Fitness of Histidine Protonation States in PDB Structures. Journal of Physical Chemistry B, 2004, 108, 12252-12257.	1.2	10
88	Reformulating the entropic contribution in molecular docking scoring functions. Journal of Computational Chemistry, 2016, 37, 1819-1827.	1.5	10
89	SAMPL6 blind predictions of water-octanol partition coefficients using nonequilibrium alchemical approaches. Journal of Computer-Aided Molecular Design, 2020, 34, 371-384.	1.3	10
90	Mounting evidence of FKBP12 implication in neurodegeneration. Neural Regeneration Research, 2020, 15, 2195.	1.6	10

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91	Comment on â€œFrom Subtle to Substantial:Â Role of Metal Ions on Ï€âˆ’Ï€ Interactionsâ€• Journal of Physical Chemistry B, 2006, 110, 10204-10205.	1.2	9
92	Free Energy Reconstruction in Bidirectional Force Spectroscopy Experiments: The Effect of the Device Stiffness. Journal of Physical Chemistry B, 2010, 114, 2509-2516.	1.2	9
93	Evidence of a Lowâ€“High Density Turning Point in Liquid Water at Ordinary Temperature under Pressure: A Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2019, 10, 6414-6418.	2.1	9
94	Imidazole in Aqueous Solution: Hydrogen Bond Interactions and Structural Reorganization with Concentration. Journal of Physical Chemistry B, 2019, 123, 4055-4064.	1.2	9
95	Binding free energy predictions in host-guest systems using Autodock4. A retrospective analysis on SAMPL6, SAMPL7 and SAMPL8 challenges. Journal of Computer-Aided Molecular Design, 2021, 35, 721-729.	1.3	9
96	SAMPL9 blind predictions using nonequilibrium alchemical approaches. Journal of Chemical Physics, 2022, 156, 164104.	1.2	9
97	Thermodynamics of stacking interactions in proteins. Annual Reports on the Progress of Chemistry Section C, 2011, 107, 242.	4.4	8
98	The conformational landscape of tartrate-based inhibitors of the TACE enzyme as revealed by Hamiltonian Replica Exchange simulation. Physical Chemistry Chemical Physics, 2013, 15, 9186.	1.3	8
99	Comment to â€œCalculation of the Dipole Moment for Polypeptides Using the Generalized Born-Electronegativity Equalization Method:Â Results in Vacuum and Continuum-Dielectric Solventâ€• Journal of Physical Chemistry B, 2004, 108, 16995-16997.	1.2	7
100	Vibrational relaxation in crystal SO2. Chemical Physics, 1991, 154, 331-342.	0.9	6
101	Comment on â€œEfficient stress relaxation in molecular dynamics simulations of semiflexiblen-alkanesâ€• [Phys. Rev. E.58, 6766 (1998)]. Physical Review E, 2001, 63, 028701; author reply 028702.	0.8	6
102	Comment on â€œClassical polarizable force fields parametrized from ab initio calculationsâ€•[J. Chem. Phys. 117, 1416 (2002)]. Journal of Chemical Physics, 2003, 118, 1571-1572.	1.2	6
103	Chiral/ring closed vs. achiral/open chain triazine-based organogelators: induction and amplification of supramolecular chirality in organic gels. Soft Matter, 2014, 10, 3762.	1.2	6
104	Polar phonons in SO2 single crystal. Chemical Physics, 1991, 151, 205-217.	0.9	5
105	Problems in molecular dynamics of condensed phases. Theoretical Chemistry Accounts, 2007, 117, 1105-1120.	0.5	5
106	Insights into the Conformational Switching Mechanism of the Human Vascular Endothelial Growth Factor Receptor Type 2 Kinase Domain. Journal of Chemical Information and Modeling, 2012, 52, 483-491.	2.5	5
107	Chemicalâ€“physical analysis of a tartrate model compound for TACE inhibition. Physical Chemistry Chemical Physics, 2013, 15, 18881.	1.3	5
108	Comment on â€œStatistical efficiency of methods for computing free energy of hydrationâ€•[J. Chem. Phys. 149, 144111 (2018)]. Journal of Chemical Physics, 2019, 150, 127101.	1.2	5

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109	Lipid tempering simulation of model biological membranes on parallel platforms. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1480-1488.	1.4	4
110	Blocking the FKBP12 induced dendrimeric burst in aberrant aggregation of Î±-synuclein by using the ElteN378 synthetic inhibitor. Journal of Enzyme Inhibition and Medicinal Chemistry, 2019, 34, 1711-1715.	2.5	4
111	A remark on the efficiency of the double-system/single-box nonequilibrium approach in the SAMPL6 SAMPLing challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 635-639.	1.3	4
112	On the NS-DSSB unidirectional estimates in the SAMPL6 SAMPLing challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 1055-1065.	1.3	4
113	Does Hamiltonian Replica Exchange via Lambda-Hopping Enhance the Sampling in Alchemical Free Energy Calculations?. Molecules, 2022, 27, 4426.	1.7	4
114	Empirical force field for the simulation of a class of chromophores in a photosynthetic center. Computational Materials Science, 2001, 20, 318-324.	1.4	3
115	Fragment 101â^'108 of Myelin Oligodendrocyte Glycoprotein: A Possible Lead Compound for Multiple Sclerosis. Journal of the American Chemical Society, 2009, 131, 17176-17184.	6.6	3
116	Media effects in modulating the conformational equilibrium of a model compound for tumor necrosis factor converting enzyme inhibition. Journal of Molecular Structure, 2015, 1091, 65-73.	1.8	3
117	Relative Binding Free Energy between Chemically Distant Compounds Using a Bidirectional Nonequilibrium Approach. Journal of Chemical Theory and Computation, 2022, 18, 4014-4026.	2.3	3
118	Computer-Aided Series Expansion for Phonon Self-Energy. Journal of Computational Physics, 2000, 165, 428-436.	1.9	1
119	Conformational structure of the MOG-derived peptide 101-108 in solution. Biopolymers, 2011, 96, 245-251.	1.2	1
120	Vibronic interactions in the lowest excited singlet state of C60. Journal of Molecular Structure, 1993, 294, 57-60.	1.8	0
121	Modeling the solvent effect in electronic transitions. , 1998, , .		0
122	Correspondence between light-absorption spectrum and nonequilibrium work distribution as a mean to access free energy differences between electronic states. Journal of Chemical Physics, 2018, 149, 084101.	1.2	0
123	Multiple Time Steps Algorithms for the Atomistic Simulations of Complex Molecular Systems. , 2000, , 333-387.		0