Piero Procacci

List of Publications by Citations

120 papers	3,502 citations	34 h-index	55 g-index
128 ext. papers	3,810 ext. citations	4.2 avg, IF	5.9 L-index

#	Paper	IF	Citations
120	Stacking and T-shape competition in aromatic-aromatic amino acid interactions. *Journal of the American Chemical Society*, **2002**, 124, 6133-43	16.4	207
119	ORAC: A Molecular dynamics program to simulate complex molecular systems with realistic electrostatic interactions. *Journal of Computational Chemistry*, **1997**, 18, 1848-1862	3.5	152
118	Glycerol condensed phases Part II.A molecular dynamics study of the conformational structure and hydrogen bonding. *Physical Chemistry Chemical Physics*, **1999**, 1, 879-885	3.6	120
117	A transferable polarizable electrostatic force field for molecular mechanics based on the chemical potential equalization principle. *Journal of Chemical Physics*, **2002**, 117, 9175-9189	3.9	119
116	Electrical response in chemical potential equalization schemes. *Journal of Chemical Physics*, **1999**, 111, 8569-8575	3.9	104
115	Glycerol condensed phases Part I. A molecular dynamics study. *Physical Chemistry Chemical Physics*, **1999**, 1, 871-877	3.6	103
114	Self-healing umbrella sampling: a non-equilibrium approach for quantitative free energy calculations. *Journal of Physical Chemistry B*, **2006**, 110, 14011-3	3.4	101
113	Identification of potential binders of the main protease 3CL of the COVID-19 via structure-based ligand design and molecular modeling. *Chemical Physics Letters*, **2020**, 750, 137489	2.5	100
112	Metadynamics simulation of prion protein: beta-structure stability and the early stages of misfolding. *Journal of the American Chemical Society*, **2006**, 128, 2705-10	16.4	93
111	Coordinates scaling and multiple time step algorithms for simulation of solvated proteins in the NPT ensemble. *Journal of Chemical Physics*, **1998**, 109, 5194-5202	3.9	88
110	A Very Fast Molecular Dynamics Method To Simulate Biomolecular Systems with Realistic Electrostatic Interactions. *The Journal of Physical Chemistry*, **1996**, 100, 10464-10468		82
109	Thermodynamics of stacking interactions in proteins. *Physical Chemistry Chemical Physics*, **2008**, 10, 2673-85	3.6	70
108	Key role of the polarization anisotropy of water in modeling classical polarizable force fields. *Journal of Physical Chemistry A*, **2007**, 111, 8170-6	2.8	70
107	The nature of intermolecular interactions between aromatic amino acid residues. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 117-25	4.2	68
106	An ab initio force field for the cofactors of bacterial photosynthesis. *Journal of Computational Chemistry*, **2003**, 24, 129-42	3.5	68
105	Calculation of optical spectra in liquid methanol using molecular dynamics and the chemical potential equalization method. *Journal of Chemical Physics*, **1999**, 111, 4218-4229	3.9	65
104	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	3.9	62

103	. *Journal of Computational Chemistry*, **1997**, 18, 1848	3.5	62
102	Density Functional Calculation of Structural and Vibrational Properties of Glycerol. *Journal of Physical Chemistry A*, **2000**, 104, 5351-5357	2.8	57
101	Simulated structure, dynamics, and vibrational spectra of liquid benzene. *Journal of Chemical Physics*, **2000**, 113, 6851-6863	3.9	57
100	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	6.4	54
99	Misfolding pathways of the prion protein probed by molecular dynamics simulations. *Biophysical Journal*, **2005**, 88, 1334-43	2.9	54
98	Crooks equation for steered molecular dynamics using a Nos□Hoover thermostat. *Journal of Chemical Physics*, **2006**, 125, 164101	3.9	52
97	ORAC: a molecular dynamics simulation program to explore free energy surfaces in biomolecular systems at the atomistic level. *Journal of Computational Chemistry*, **2010**, 31, 1106-16	3.5	50
96	Electrostatic calculations and multiple time scales in molecular dynamics simulation of flexible molecular systems. *Journal of Chemical Physics*, **1998**, 108, 8799-8803	3.9	46
95	Computer simulation of solid C60 using multiple time-step algorithms. *Journal of Chemical Physics*, **1994**, 101, 2421-2431	3.9	43
94	Multiple time scale methods for constant pressure molecular dynamics simulations of molecular systems. *Molecular Physics*, **1994**, 83, 255-272	1.7	42
93	Interaction between Aromatic Residues. Molecular Dynamics and ab Initio Exploration of the Potential Energy Surface of the Tryptophan□Histidine Pair. *Journal of Physical Chemistry B*, **2000**, 104, 1108-1114	3.4	40
92	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	3.9	36
91	Is the T-Shaped Toluene Dimer a Stable Intermolecular Complex?. *Journal of Physical Chemistry A*, **2002**, 106, 2945-2948	2.8	36
90	Statistical Mechanics of Ligand-Receptor Noncovalent Association, Revisited: Binding Site and Standard State Volumes in Modern Alchemical Theories. *Journal of Chemical Theory and Computation*, **2017**, 13, 1924-1933	6.4	34
89	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, 1117-21	6.1	34
88	A potential of mean force estimator based on nonequilibrium work exponential averages. *Physical Chemistry Chemical Physics*, **2009**, 11, 1152-8	3.6	34
87	Generalization of the Jarzynski and Crooks nonequilibrium work theorems in molecular dynamics simulations. *Physical Review E*, **2007**, 75, 050101	2.4	34
86	Comparing polarizable force fields to ab initio calculations reveals nonclassical effects in condensed phases. *Journal of Chemical Physics*, **2005**, 122, 234107	3.9	34

85	Calculation of the potential of mean force from nonequilibrium measurements via maximum likelihood estimators. *Physical Review E*, **2008**, 77, 031104	2.4	32
84	Conformational Distribution of Gas-phase Glycerol. *Journal of Physical Chemistry A*, **2000**, 104, 11220-11228	2.8	32
83	Fast Switching Alchemical Transformations in Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 2813-23	6.4	31
82	Efficient nonequilibrium method for binding free energy calculations in molecular dynamics simulations. *Journal of Chemical Theory and Computation*, **2015**, 11, 423-35	6.4	31
81	A general algorithm for computing Voronoi volumes: Application to the hydrated crystal of myoglobin. *International Journal of Quantum Chemistry*, **1992**, 42, 1515-1528	2.1	31
80	Anharmonic calculation of bandwidths and frequency shifts in crystalline CO2. *Chemical Physics*, **1987**, 116, 171-186	2.3	31
79	Vibrational frequencies of C70. *Chemical Physics Letters*, **1992**, 195, 347-351	2.5	30
78	II. Dissociation free energies in drug-receptor systems via nonequilibrium alchemical simulations: application to the FK506-related immunophilin ligands. *Physical Chemistry Chemical Physics*, **2016**, 18, 15005-18	3.6	30
77	Determination of the Potential of Mean Force of Aromatic Amino Acid Complexes in Various Solvents Using Molecular Dynamics Simulations:´The Case of the Tryptophan−Histidine Pair. *Journal of Physical Chemistry B*, **2001**, 105, 7835-7846	3.4	28
76	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	6.1	27
75	SAMPL6 host-guest blind predictions using a non equilibrium alchemical approach. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 965-982	4.2	26
74	I. Dissociation free energies of drug-receptor systems via non-equilibrium alchemical simulations: a theoretical framework. *Physical Chemistry Chemical Physics*, **2016**, 18, 14991-5004	3.6	26
73	The precise chemical-physical nature of the pharmacore in FK506 binding protein inhibition: ElteX, a New class of nanomolar FKBP12 ligands. *Journal of Medicinal Chemistry*, **2013**, 56, 1041-51	8.3	25
72	Vibrational properties of Xe−fullerene adducts. A molecular dynamics approach. *Chemical Physics Letters*, **1992**, 200, 39-45	2.5	22
71	Unbiased free energy estimates in fast nonequilibrium transformations using Gaussian mixtures. *Journal of Chemical Physics*, **2015**, 142, 154117	3.9	21
70	Hummer and Szabo-like potential of mean force estimator for bidirectional nonequilibrium pulling experiments/simulations. *Journal of Physical Chemistry B*, **2010**, 114, 9546-54	3.4	19
69	The far-infrared spectrum of crystalline fullerene C60. *The Journal of Physical Chemistry*, **1993**, 97, 10580-10584	2.8	19
68	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	6.1	18

67	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	6.4	18
66	Interaction of hydroxychloroquine with SARS-CoV2 functional proteins using all-atoms non-equilibrium alchemical simulations. *Chemical Communications*, **2020**, 56, 8854-8856	5.8	17
65	Regioselective electrophilic access to naphtho[1,2-b:8,7-b']- and -[1,2-b:5,6-b']dithiophenes. *Journal of Organic Chemistry*, **2013**, 78, 3496-502	4.2	17
64	Towards a polarizable force field for molecular liquids. *Journal of Molecular Liquids*, **2002**, 96-97, 87-100	6	17
63	Molecular dynamics of glass-forming liquids: Structure and dynamics of liquid metatoluidine. *Journal of Chemical Physics*, **2002**, 116, 6205-6215	3.9	17
62	Anharmonic lattice dynamics and computer simulation for simple model systems. *Physical Review B*, **1992**, 45, 2113-2125	3.3	17
61	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	2.8	15
60	New Perspective on How and Why Immunophilin FK506-Related Ligands Work. *Journal of Physical Chemistry Letters*, **2011**, 2, 2834-2839	6.4	15
59	Numerical verification of the generalized Crooks nonequilibrium work theorem for non-Hamiltonian molecular dynamics simulations. *Journal of Chemical Physics*, **2007**, 127, 034110	3.9	14
58	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	2.8	14
57	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	6.4	13
56	Energy dissipation asymmetry in the non equilibrium folding/unfolding of the single molecule alanine decapeptide. *Chemical Physics*, **2010**, 375, 8-15	2.3	13
55	Inter-residue and solvent-residue interactions in proteins: a statistical study on experimental structures. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 139-51	4.2	13
54	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	3.9	13
53	Molecular dynamics and anharmonic effects in the phonon spectra of solid carbon dioxide. *Chemical Physics*, **1987**, 117, 355-366	2.3	13
52	Solvation free energies via alchemical simulations: let's get honest about sampling, once more. *Physical Chemistry Chemical Physics*, **2019**, 21, 13826-13834	3.6	12
51	Energy-Driven Undocking (EDU-HREM) in Solute Tempering Replica Exchange Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 439-50	6.4	12
50	Conformational landscape of N-glycosylated peptides detecting autoantibodies in multiple sclerosis, revealed by Hamiltonian replica exchange. *Journal of Physical Chemistry B*, **2012**, 116, 5458-67	3.4	12

49	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	3.9	12
48	Equation of motion for the Green's function in anharmonic solids. *Physical Review B*, **1992**, 46, 6141-6149	3.3	12
47	Intraligand hydrophobic interactions rationalize drug affinities for peptidyl-prolyl cis-trans isomerase protein. *Journal of Physical Chemistry B*, **2011**, 115, 6193-201	3.4	11
46	Dynamical and structural correlation in supercooled liquids: A molecular dynamics investigation of m-toluidine. *Journal of Chemical Physics*, **2003**, 119, 357-363	3.9	11
45	Multiple Bennett acceptance ratio made easy for replica exchange simulations. *Journal of Chemical Physics*, **2013**, 139, 124105	3.9	10
44	Energetic Fitness of Histidine Protonation States in PDB Structures. *Journal of Physical Chemistry B*, **2004**, 108, 12252-12257	3.4	10
43	Efficient calculation of high-order self-energy corrections to phonon linewidths: Application to alpha -nitrogen. *Physical Review B*, **1993**, 47, 11124-11133	3.3	10
42	Accuracy, precision, and efficiency of nonequilibrium alchemical methods for computing free energies of solvation. I. Bidirectional approaches. *Journal of Chemical Physics*, **2019**, 151, 144113	3.9	10
41	Precision and computational efficiency of nonequilibrium alchemical methods for computing free energies of solvation. II. Unidirectional estimates. *Journal of Chemical Physics*, **2019**, 151, 144115	3.9	10
40	Mycotoxins aptasensing: From molecular docking to electrochemical detection of deoxynivalenol. *Bioelectrochemistry*, **2021**, 138, 107691	5.6	10
39	Binding Free Energies of Host-Guest Systems by Nonequilibrium Alchemical Simulations with Constrained Dynamics: Theoretical Framework. *Journal of Chemical Theory and Computation*, **2017**, 13, 5874-5886	6.4	9
38	Comment on "from subtle to substantial: role of metal ions on pi-pi interactions". *Journal of Physical Chemistry B*, **2006**, 110, 10204-5; discussion 10206-7	3.4	9
37	SAMPL6 blind predictions of water-octanol partition coefficients using nonequilibrium alchemical approaches. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 371-384	4.2	9
36	Imidazole in Aqueous Solution: Hydrogen Bond Interactions and Structural Reorganization with Concentration. *Journal of Physical Chemistry B*, **2019**, 123, 4055-4064	3.4	8
35	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	3.9	8
34	Binding Free Energies of Host-Guest Systems by Nonequilibrium Alchemical Simulations with Constrained Dynamics: Illustrative Calculations and Numerical Validation. *Journal of Chemical Theory and Computation*, **2017**, 13, 5887-5899	6.4	8
33	Free energy reconstruction in bidirectional force spectroscopy experiments: the effect of the device stiffness. *Journal of Physical Chemistry B*, **2010**, 114, 2509-16	3.4	8
32	Thermodynamics of stacking interactions in proteins. *Annual Reports on the Progress of Chemistry Section C*, **2011**, 107, 242		7

31	Comment to Calculation of the Dipole Moment for Polypeptides Using the Generalized Born-Electronegativity Equalization Method: Results in Vacuum and Continuum-Dielectric Solvent. *Journal of Physical Chemistry B*, **2004**, 108, 16995-16997	3.4	7
30	Methodological uncertainties in drug-receptor binding free energy predictions based on classical molecular dynamics. *Current Opinion in Structural Biology*, **2021**, 67, 127-134	8.1	7
29	SAMPL7 blind predictions using nonequilibrium alchemical approaches. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 37-47	4.2	7
28	Evidence of a Low-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	6.4	6
27	Comment on Classical polarizable force fields parametrized from ab initio calculations [J. Chem. Phys. 117, 1416 (2002)]. *Journal of Chemical Physics*, **2003**, 118, 1571-1572	3.9	6
26	Vibrational relaxation in crystal SO2. *Chemical Physics*, **1991**, 154, 331-342	2.3	6
25	Reformulating the entropic contribution in molecular docking scoring functions. *Journal of Computational Chemistry*, **2016**, 37, 1819-27	3.5	6
24	Comment on "Statistical efficiency of methods for computing free energy of hydration" [J. Chem. Phys. 149, 144111 (2018)]. *Journal of Chemical Physics*, **2019**, 150, 127101	3.9	5
23	Chiral/ring closed vs. achiral/open chain triazine-based organogelators: induction and amplification of supramolecular chirality in organic gels. *Soft Matter*, **2014**, 10, 3762-70	3.6	5
22	The conformational landscape of tartrate-based inhibitors of the TACE enzyme as revealed by Hamiltonian Replica Exchange simulation. *Physical Chemistry Chemical Physics*, **2013**, 15, 9186-96	3.6	5
21	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, 483-91	6.1	5
20	Chemical-physical analysis of a tartrate model compound for TACE inhibition. *Physical Chemistry Chemical Physics*, **2013**, 15, 18881-93	3.6	5
19	Problems in molecular dynamics of condensed phases. *Theoretical Chemistry Accounts*, **2007**, 117, 1105-1120	1.9	5
18	Comment on "Efficient stress relaxation in molecular dynamics simulations of semiflexible n-alkanes". *Physical Review E*, **2001**, 63, 028701; author reply 028702	2.4	5
17	Polar phonons in SO2 single crystal. *Chemical Physics*, **1991**, 151, 205-217	2.3	5
16	Mounting evidence of FKBP12 implication in neurodegeneration. *Neural Regeneration Research*, **2020**, 15, 2195-2202	4.5	4
15	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	3.4	3
14	Lipid tempering simulation of model biological membranes on parallel platforms. *Biochimica Et Biophysica Acta - Biomembranes*, **2018**, 1860, 1480-1488	3.8	3

13	Empirical force field for the simulation of a class of chromophores in a photosynthetic center. *Computational Materials Science*, **2001**, 20, 318-324	3.2	3
12	On the NS-DSSB unidirectional estimates in the SAMPL6 SAMPLing challenge. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 1055-1065	4.2	3
11	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	4.2	3
10	Fragment 101-108 of myelin oligodendrocyte glycoprotein: a possible lead compound for multiple sclerosis. *Journal of the American Chemical Society*, **2009**, 131, 17176-84	16.4	2
9	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	4.2	2
8	Blocking the FKBP12 induced dendrimeric burst in aberrant aggregation of α-synuclein by using the ElteN378 synthetic inhibitor. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2019**, 34, 1711-1715	5.6	1
7	Conformational structure of the MOG-derived peptide 101-108 in solution. *Biopolymers*, **2011**, 96, 245-51	2.2	1
6	Computer-Aided Series Expansion for Phonon Self-Energy. *Journal of Computational Physics*, **2000**, 165, 428-436	4.1	1
5	Virtual Double-System Single-Box for Absolute Dissociation Free Energy Calculations in GROMACS. *Journal of Chemical Information and Modeling*, **2021**, 61, 5320-5326	6.1	1
4	SAMPL9 blind predictions using nonequilibrium alchemical approaches.. *Journal of Chemical Physics*, **2022**, 156, 164104	3.9	0
3	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	3.9	
2	Vibronic interactions in the lowest excited singlet state of C60. *Journal of Molecular Structure*, **1993** , 294, 57-60	3.4	
1	Multiple Time Steps Algorithms for the Atomistic Simulations of Complex Molecular Systems **2000**, 333-387		