

Piero Procacci

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Characterization of the non-covalent interaction between the PF-07321332 inhibitor and the SARS-CoV-2 main protease. <i>Journal of Molecular Graphics and Modelling</i> , 2022 , 110, 108042	2.8	14
119	SAMPL9 blind predictions using nonequilibrium alchemical approaches.. <i>Journal of Chemical Physics</i> , 2022 , 156, 164104	3.9	0
118	On the NS-DSSB unidirectional estimates in the SAMPL6 SAMPLing challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2021 , 35, 1055-1065	4.2	3
117	Virtual Double-System Single-Box for Absolute Dissociation Free Energy Calculations in GROMACS. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 5320-5326	6.1	1
116	Binding free energy predictions in host-guest systems using Autodock4. A retrospective analysis on SAMPL6, SAMPL7 and SAMPL8 challenges. <i>Journal of Computer-Aided Molecular Design</i> , 2021 , 35, 721-729	4.2	2
115	Mycotoxins aptasensing: From molecular docking to electrochemical detection of deoxynivalenol. <i>Bioelectrochemistry</i> , 2021 , 138, 107691	5.6	10
114	Methodological uncertainties in drug-receptor binding free energy predictions based on classical molecular dynamics. <i>Current Opinion in Structural Biology</i> , 2021 , 67, 127-134	8.1	7
113	SAMPL7 blind predictions using nonequilibrium alchemical approaches. <i>Journal of Computer-Aided Molecular Design</i> , 2021 , 35, 37-47	4.2	7
112	Upgraded AMBER Force Field for Zinc-Binding Residues and Ligands for Predicting Structural Properties and Binding Affinities in Zinc-Proteins. <i>ACS Omega</i> , 2020 , 5, 15301-15310	3.9	8
111	Interaction of hydroxychloroquine with SARS-CoV2 functional proteins using all-atoms non-equilibrium alchemical simulations. <i>Chemical Communications</i> , 2020 , 56, 8854-8856	5.8	17
110	Mounting evidence of FKBP12 implication in neurodegeneration. <i>Neural Regeneration Research</i> , 2020 , 15, 2195-2202	4.5	4
109	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. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 7160-7172	6.4	18
108	SAMPL6 blind predictions of water-octanol partition coefficients using nonequilibrium alchemical approaches. <i>Journal of Computer-Aided Molecular Design</i> , 2020 , 34, 371-384	4.2	9
107	A remark on the efficiency of the double-system/single-box nonequilibrium approach in the SAMPL6 SAMPLing challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2020 , 34, 635-639	4.2	3
106	Identification of potential binders of the main protease 3CL of the COVID-19 via structure-based ligand design and molecular modeling. <i>Chemical Physics Letters</i> , 2020 , 750, 137489	2.5	100
105	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. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 1983-1995	6.4	54
104	Solvation free energies via alchemical simulations: let's get honest about sampling, once more. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 13826-13834	3.6	12

103	Comment on "Statistical efficiency of methods for computing free energy of hydration" [J. Chem. Phys. 149, 144111 (2018)]. <i>Journal of Chemical Physics</i> , 2019 , 150, 127101	3.9	5
102	Imidazole in Aqueous Solution: Hydrogen Bond Interactions and Structural Reorganization with Concentration. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 4055-4064	3.4	8
101	Upgrading and Validation of the AMBER Force Field for Histidine and Cysteine Zinc(II)-Binding Residues in Sites with Four Protein Ligands. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 3803-3816 ¹⁸	6.1	18
100	Blocking the FKBP12 induced dendrimeric burst in aberrant aggregation of β -synuclein by using the ElteN378 synthetic inhibitor. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2019 , 34, 1711-1715	5.6	1
99	Evidence of a Low-High Density Turning Point in Liquid Water at Ordinary Temperature under Pressure: A Molecular Dynamics Study. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 6414-6418	6.4	6
98	Accuracy, precision, and efficiency of nonequilibrium alchemical methods for computing free energies of solvation. I. Bidirectional approaches. <i>Journal of Chemical Physics</i> , 2019 , 151, 144113	3.9	10
97	Precision and computational efficiency of nonequilibrium alchemical methods for computing free energies of solvation. II. Unidirectional estimates. <i>Journal of Chemical Physics</i> , 2019 , 151, 144115	3.9	10
96	Lipid tempering simulation of model biological membranes on parallel platforms. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018 , 1860, 1480-1488	3.8	3
95	Correspondence between light-absorption spectrum and nonequilibrium work distribution as a mean to access free energy differences between electronic states. <i>Journal of Chemical Physics</i> , 2018 , 149, 084101	3.9	
94	SAMPL6 host-guest blind predictions using a non equilibrium alchemical approach. <i>Journal of Computer-Aided Molecular Design</i> , 2018 , 32, 965-982	4.2	26
93	Myeloid Cell Leukemia 1 Inhibition: An in Silico Study Using Non-equilibrium Fast Double Annihilation Technology. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 3890-3902	6.4	13
92	Alchemical determination of drug-receptor binding free energy: Where we stand and where we could move to. <i>Journal of Molecular Graphics and Modelling</i> , 2017 , 71, 233-241	2.8	15
91	PrimaDORAC: A Free Web Interface for the Assignment of Partial Charges, Chemical Topology, and Bonded Parameters in Organic or Drug Molecules. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 1240-1245	6.1	27
90	Statistical Mechanics of Ligand-Receptor Noncovalent Association, Revisited: Binding Site and Standard State Volumes in Modern Alchemical Theories. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 1924-1933	6.4	34
89	Binding Free Energies of Host-Guest Systems by Nonequilibrium Alchemical Simulations with Constrained Dynamics: Theoretical Framework. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 5874-5886	6.4	9
88	Binding Free Energies of Host-Guest Systems by Nonequilibrium Alchemical Simulations with Constrained Dynamics: Illustrative Calculations and Numerical Validation. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 5887-5899	6.4	8
87	Hybrid MPI/OpenMP Implementation of the ORAC Molecular Dynamics Program for Generalized Ensemble and Fast Switching Alchemical Simulations. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 1117-21	6.1	34
86	Reformulating the entropic contribution in molecular docking scoring functions. <i>Journal of Computational Chemistry</i> , 2016 , 37, 1819-27	3.5	6

85	I. Dissociation free energies of drug-receptor systems via non-equilibrium alchemical simulations: a theoretical framework. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 14991-5004	3.6	26
84	II. Dissociation free energies in drug-receptor systems via nonequilibrium alchemical simulations: application to the FK506-related immunophilin ligands. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 15005-18	3.6	30
83	Unbiased free energy estimates in fast nonequilibrium transformations using Gaussian mixtures. <i>Journal of Chemical Physics</i> , 2015 , 142, 154117	3.9	21
82	Media effects in modulating the conformational equilibrium of a model compound for tumor necrosis factor converting enzyme inhibition. <i>Journal of Molecular Structure</i> , 2015 , 1091, 65-73	3.4	3
81	Efficient nonequilibrium method for binding free energy calculations in molecular dynamics simulations. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 423-35	6.4	31
80	Energy-Driven Undocking (EDU-HREM) in Solute Tempering Replica Exchange Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 439-50	6.4	12
79	Fast Switching Alchemical Transformations in Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2813-23	6.4	31
78	Chiral/ring closed vs. achiral/open chain triazine-based organogelators: induction and amplification of supramolecular chirality in organic gels. <i>Soft Matter</i> , 2014 , 10, 3762-70	3.6	5
77	The conformational landscape of tartrate-based inhibitors of the TACE enzyme as revealed by Hamiltonian Replica Exchange simulation. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 9186-96	3.6	5
76	The precise chemical-physical nature of the pharmacore in FK506 binding protein inhibition: ElteX, a New class of nanomolar FKBP12 ligands. <i>Journal of Medicinal Chemistry</i> , 2013 , 56, 1041-51	8.3	25
75	Regioselective electrophilic access to naphtho[1,2-b:8,7-b']- and -[1,2-b:5,6-b']dithiophenes. <i>Journal of Organic Chemistry</i> , 2013 , 78, 3496-502	4.2	17
74	Chemical-physical analysis of a tartrate model compound for TACE inhibition. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 18881-93	3.6	5
73	Multiple Bennett acceptance ratio made easy for replica exchange simulations. <i>Journal of Chemical Physics</i> , 2013 , 139, 124105	3.9	10
72	Conformational landscape of N-glycosylated peptides detecting autoantibodies in multiple sclerosis, revealed by Hamiltonian replica exchange. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 5458-67	3.4	12
71	Insights into the conformational switching mechanism of the human vascular endothelial growth factor receptor type 2 kinase domain. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 483-91	6.1	5
70	Thermodynamics of stacking interactions in proteins. <i>Annual Reports on the Progress of Chemistry Section C</i> , 2011 , 107, 242		7
69	Conformational structure of the MOG-derived peptide 101-108 in solution. <i>Biopolymers</i> , 2011 , 96, 245-51	5.2	1
68	Intraligand hydrophobic interactions rationalize drug affinities for peptidyl-prolyl cis-trans isomerase protein. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 6193-201	3.4	11

67	New Perspective on How and Why Immunophilin FK506-Related Ligands Work. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 2834-2839	6.4	15
66	Free energy reconstruction in bidirectional force spectroscopy experiments: the effect of the device stiffness. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 2509-16	3.4	8
65	Hummer and Szabo-like potential of mean force estimator for bidirectional nonequilibrium pulling experiments/simulations. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 9546-54	3.4	19
64	ORAC: a molecular dynamics simulation program to explore free energy surfaces in biomolecular systems at the atomistic level. <i>Journal of Computational Chemistry</i> , 2010 , 31, 1106-16	3.5	50
63	Energy dissipation asymmetry in the non equilibrium folding/unfolding of the single molecule alanine decapeptide. <i>Chemical Physics</i> , 2010 , 375, 8-15	2.3	13
62	Fragment 101-108 of myelin oligodendrocyte glycoprotein: a possible lead compound for multiple sclerosis. <i>Journal of the American Chemical Society</i> , 2009 , 131, 17176-84	16.4	2
61	A potential of mean force estimator based on nonequilibrium work exponential averages. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 1152-8	3.6	34
60	Thermodynamics of stacking interactions in proteins. <i>Physical Chemistry Chemical Physics</i> , 2008 , 10, 2673-85	3.85	70
59	Calculation of the potential of mean force from nonequilibrium measurements via maximum likelihood estimators. <i>Physical Review E</i> , 2008 , 77, 031104	2.4	32
58	Key role of the polarization anisotropy of water in modeling classical polarizable force fields. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 8170-6	2.8	70
57	Recovering the Crooks equation for dynamical systems in the isothermal-isobaric ensemble: a strategy based on the equations of motion. <i>Journal of Chemical Physics</i> , 2007 , 126, 044502	3.9	12
56	Problems in molecular dynamics of condensed phases. <i>Theoretical Chemistry Accounts</i> , 2007 , 117, 1105-1120	3.0	5
55	Numerical verification of the generalized Crooks nonequilibrium work theorem for non-Hamiltonian molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2007 , 127, 034110	3.9	14
54	Generalization of the Jarzynski and Crooks nonequilibrium work theorems in molecular dynamics simulations. <i>Physical Review E</i> , 2007 , 75, 050101	2.4	34
53	Crooks equation for steered molecular dynamics using a Nosé-Hoover thermostat. <i>Journal of Chemical Physics</i> , 2006 , 125, 164101	3.9	52
52	Self-healing umbrella sampling: a non-equilibrium approach for quantitative free energy calculations. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 14011-3	3.4	101
51	Metadynamics simulation of prion protein: beta-structure stability and the early stages of misfolding. <i>Journal of the American Chemical Society</i> , 2006 , 128, 2705-10	16.4	93
50	Comment on "from subtle to substantial: role of metal ions on pi-pi interactions". <i>Journal of Physical Chemistry B</i> , 2006 , 110, 10204-5; discussion 10206-7	3.4	9

49	Misfolding pathways of the prion protein probed by molecular dynamics simulations. <i>Biophysical Journal</i> , 2005 , 88, 1334-43	2.9	54
48	Polarization response of water and methanol investigated by a polarizable force field and density functional theory calculations: implications for charge transfer. <i>Journal of Chemical Physics</i> , 2005 , 122, 074504	3.9	36
47	Behavior of polarizable models in presence of strong electric fields. I. Origin of nonlinear effects in water point-charge systems. <i>Journal of Chemical Physics</i> , 2005 , 123, 194109	3.9	13
46	Comparing polarizable force fields to ab initio calculations reveals nonclassical effects in condensed phases. <i>Journal of Chemical Physics</i> , 2005 , 122, 234107	3.9	34
45	Inter-residue and solvent-residue interactions in proteins: a statistical study on experimental structures. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004 , 55, 139-51	4.2	13
44	Comment to "Calculation of the Dipole Moment for Polypeptides Using the Generalized Born-Electronegativity Equalization Method: Results in Vacuum and Continuum-Dielectric Solvent" <i>Journal of Physical Chemistry B</i> , 2004 , 108, 16995-16997	3.4	7
43	Energetic Fitness of Histidine Protonation States in PDB Structures. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 12252-12257	3.4	10
42	Comment on "Classical polarizable force fields parametrized from ab initio calculations" [<i>J. Chem. Phys.</i> 117, 1416 (2002)]. <i>Journal of Chemical Physics</i> , 2003 , 118, 1571-1572	3.9	6
41	An ab initio force field for the cofactors of bacterial photosynthesis. <i>Journal of Computational Chemistry</i> , 2003 , 24, 129-42	3.5	68
40	Dynamical and structural correlation in supercooled liquids: A molecular dynamics investigation of m-toluidine. <i>Journal of Chemical Physics</i> , 2003 , 119, 357-363	3.9	11
39	Towards a polarizable force field for molecular liquids. <i>Journal of Molecular Liquids</i> , 2002 , 96-97, 87-100	6	17
38	The nature of intermolecular interactions between aromatic amino acid residues. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002 , 48, 117-25	4.2	68
37	Is the T-Shaped Toluene Dimer a Stable Intermolecular Complex?. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 2945-2948	2.8	36
36	Molecular dynamics of glass-forming liquids: Structure and dynamics of liquid metatoluidine. <i>Journal of Chemical Physics</i> , 2002 , 116, 6205-6215	3.9	17
35	A transferable polarizable electrostatic force field for molecular mechanics based on the chemical potential equalization principle. <i>Journal of Chemical Physics</i> , 2002 , 117, 9175-9189	3.9	119
34	Stacking and T-shape competition in aromatic-aromatic amino acid interactions. <i>Journal of the American Chemical Society</i> , 2002 , 124, 6133-43	16.4	207
33	Comment on "Efficient stress relaxation in molecular dynamics simulations of semiflexible n-alkanes". <i>Physical Review E</i> , 2001 , 63, 028701; author reply 028702	2.4	5
32	Empirical force field for the simulation of a class of chromophores in a photosynthetic center. <i>Computational Materials Science</i> , 2001 , 20, 318-324	3.2	3

31	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. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 7835-7846	3.4	28
30	Computer-Aided Series Expansion for Phonon Self-Energy. <i>Journal of Computational Physics</i> , 2000 , 165, 428-436	4.1	1
29	Interaction between Aromatic Residues. Molecular Dynamics and ab Initio Exploration of the Potential Energy Surface of the Tryptophan-Histidine Pair. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 1108-1114	3.4	40
28	Density Functional Calculation of Structural and Vibrational Properties of Glycerol. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 5351-5357	2.8	57
27	Conformational Distribution of Gas-phase Glycerol. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 11220-11222	3.2	32
26	Simulated structure, dynamics, and vibrational spectra of liquid benzene. <i>Journal of Chemical Physics</i> , 2000 , 113, 6851-6863	3.9	57
25	Multiple Time Steps Algorithms for the Atomistic Simulations of Complex Molecular Systems 2000 , 333-387		
24	Electrical response in chemical potential equalization schemes. <i>Journal of Chemical Physics</i> , 1999 , 111, 8569-8575	3.9	104
23	Calculation of optical spectra in liquid methanol using molecular dynamics and the chemical potential equalization method. <i>Journal of Chemical Physics</i> , 1999 , 111, 4218-4229	3.9	65
22	Glycerol condensed phases Part I. A molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 1999 , 1, 871-877	3.6	103
21	Glycerol condensed phases Part II. A molecular dynamics study of the conformational structure and hydrogen bonding. <i>Physical Chemistry Chemical Physics</i> , 1999 , 1, 879-885	3.6	120
20	Electrostatic calculations and multiple time scales in molecular dynamics simulation of flexible molecular systems. <i>Journal of Chemical Physics</i> , 1998 , 108, 8799-8803	3.9	46
19	Coordinates scaling and multiple time step algorithms for simulation of solvated proteins in the NPT ensemble. <i>Journal of Chemical Physics</i> , 1998 , 109, 5194-5202	3.9	88
18	ORAC: A Molecular dynamics program to simulate complex molecular systems with realistic electrostatic interactions. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1848-1862	3.5	152
17	. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1848	3.5	62
16	A Very Fast Molecular Dynamics Method To Simulate Biomolecular Systems with Realistic Electrostatic Interactions. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 10464-10468		82
15	Taming the Ewald sum in molecular dynamics simulations of solvated proteins via a multiple time step algorithm. <i>Journal of Chemical Physics</i> , 1996 , 104, 3003-3012	3.9	62
14	Multiple time scale methods for constant pressure molecular dynamics simulations of molecular systems. <i>Molecular Physics</i> , 1994 , 83, 255-272	1.7	42

- 13 Computer simulation of solid C60 using multiple time-step algorithms. *Journal of Chemical Physics*, **1994**, 101, 2421-2431 3.9 43
- 12 The far-infrared spectrum of crystalline fullerene C60. *The Journal of Physical Chemistry*, **1993**, 97, 10580-10584.9
- 11 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
- 10 Vibronic interactions in the lowest excited singlet state of C60. *Journal of Molecular Structure*, **1993**, 294, 57-60 3.4
- 9 Equation of motion for the Green's function in anharmonic solids. *Physical Review B*, **1992**, 46, 6141-6149.3 12
- 8 Anharmonic lattice dynamics and computer simulation for simple model systems. *Physical Review B*, **1992**, 45, 2113-2125 3.3 17
- 7 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
- 6 Vibrational frequencies of C70. *Chemical Physics Letters*, **1992**, 195, 347-351 2.5 30
- 5 Vibrational properties of Xe fullerene adducts. A molecular dynamics approach. *Chemical Physics Letters*, **1992**, 200, 39-45 2.5 22
- 4 Vibrational relaxation in crystal SO2. *Chemical Physics*, **1991**, 154, 331-342 2.3 6
- 3 Polar phonons in SO2 single crystal. *Chemical Physics*, **1991**, 151, 205-217 2.3 5
- 2 Molecular dynamics and anharmonic effects in the phonon spectra of solid carbon dioxide. *Chemical Physics*, **1987**, 117, 355-366 2.3 13
- 1 Anharmonic calculation of bandwidths and frequency shifts in crystalline CO2. *Chemical Physics*, **1987**, 116, 171-186 2.3 31