Riccardo Baron

List of Publications by Year
in descending order

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58	4,628	168829	150775
papers	citations	31 h-index	59 g-index

62	62	62	6428
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A marine analgesic peptide, Contulakin-G, and neurotensin are distinct agonists for neurotensin receptors: uncovering structural determinants of desensitization properties. Frontiers in Pharmacology, 2015, 6, 11.	1.6	29
2	Combined STAT3 and BCR-ABL1 inhibition induces synthetic lethality in therapy-resistant chronic myeloid leukemia. Leukemia, 2015, 29, 586-597.	3.3	111
3	Epigenetic Molecular Recognition: A Biomolecular Modeling Perspective. ChemMedChem, 2014, 9, 484-494.	1.6	9
4	PITOMBA: Parameter Interface for Oligosaccharide Molecules Based on Atoms. Journal of Chemical Theory and Computation, 2014, 10, 5068-5080.	2.3	20
5	BCR-ABL1 Compound Mutations Combining Key Kinase Domain Positions Confer Clinical Resistance to Ponatinib in Ph Chromosome-Positive Leukemia. Cancer Cell, 2014, 26, 428-442.	7.7	292
6	Coarse-Graining of TIP4P/2005, TIP4P-Ew, SPC/E, and TIP3P to Monatomic Anisotropic Water Models Using Relative Entropy Minimization. Journal of Chemical Theory and Computation, 2014, 10, 4104-4120.	2.3	108
7	MDWiZ: A platform for the automated translation of molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2014, 48, 80-86.	1.3	10
8	Design, Optimization, and Pre-Clinical Evaluation of Direct, Mechanism-Based STAT3 Inhibitors for Treating Myeloid Disorders. Blood, 2014, 124, 4816-4816.	0.6	0
9	Thiuram Disulfides as Pseudoâ€irreversible Inhibitors of Lymphoid Tyrosine Phosphatase. ChemMedChem, 2013, 8, 1561-1568.	1.6	9
10	Variational Implicit-Solvent Modeling of Hostâ€“Guest Binding: A Case Study on Cucurbit[7]uril|. Journal of Chemical Theory and Computation, 2013, 9, 4195-4204.	2.3	12
11	Fast Sampling of A-to-B Protein Global Conformational Transitions: From Galileo Galilei to Monte Carlo Anisotropic Network Modeling. Biophysical Journal, 2013, 105, 1545-1546.	0.2	2
12	Molecular dynamics simulations indicate an induced-fit mechanism for LSD1/CoREST-H3-histone molecular recognition. BMC Biophysics, 2013, 6, 15.	4.4	15
13	Substrate Selection Influences Molecular Recognition in a Screen for Lymphoid Tyrosine Phosphatase Inhibitors. ChemBioChem, 2013, 14, 1640-1647.	1.3	7
14	Solvent fluctuations in hydrophobic cavityâ€“ligand binding kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 1197-1202.	3.3	86
15	Comment on â€˜Molecular driving forces of the pocket-ligand hydrophobic associationâ€™ by G. Graziano, Chem. Phys. Lett. 533 (2012) 95. Chemical Physics Letters, 2013, 555, 306-309.	1.2	1
16	Molecular Recognition and Ligand Association. Annual Review of Physical Chemistry, 2013, 64, 151-175.	4.8	165
17	Protein Recognition by Short Peptide Reversible Inhibitors of the Chromatin-Modifying LSD1/CoREST Lysine Demethylase. ACS Chemical Biology, 2013, 8, 1677-1682.	1.6	60
18	On the Role of Dewetting Transitions in Hostâ€“Guest Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2013, 9, 46-53.	2.3	26

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19	Expanding the Druggable Space of the LSD1/CoREST Epigenetic Target: New Potential Binding Regions for Drug-Like Molecules, Peptides, Protein Partners, and Chromatin. PLoS Computational Biology, 2013, 9, e1003158.	1.5	27
20	BP5-087, a Novel STAT3 Inhibitor, Combines With BCR-ABL1 Inhibition To Overcome Kinase-Independent Resistance In Chronic Myeloid Leukemia. Blood, 2013, 122, 854-854.	0.6	0
21	LSD1/CoREST is an allosteric nanoscale clamp regulated by H3-histone-tail molecular recognition. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 12509-12514.	3.3	59
22	Water Structure, Dynamics, and Spectral Signatures: Changes Upon Model Cavityâ€“Ligand Recognition. Journal of Physical Chemistry B, 2012, 116, 13774-13780.	1.2	12
23	LSD1/CoREST Reversible Openingâ€“Closing Dynamics: Discovery of a Nanoscale Clamp for Chromatin and Protein Binding. Biochemistry, 2012, 51, 3151-3153.	1.2	19
24	Water-Driven Cavityâ€“Ligand Binding: Comparison of Thermodynamic Signatures from Coarse-Grained and Atomic-Level Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3696-3704.	2.3	46
25	Computational Drug Discovery and Design. Methods in Molecular Biology, 2012, , .	0.4	30
26	On the Use of Molecular Dynamics Receptor Conformations for Virtual Screening. Methods in Molecular Biology, 2012, 819, 93-103.	0.4	20
27	Independent-Trajectory Thermodynamic Integration: A Practical Guide to Protein-Drug Binding Free Energy Calculations Using Distributed Computing. Methods in Molecular Biology, 2012, 819, 469-486.	0.4	10
28	Predictive Power of Molecular Dynamics Receptor Structures in Virtual Screening. Journal of Chemical Information and Modeling, 2011, 51, 1439-1446.	2.5	91
29	Effects of Biomolecular Flexibility on Alchemical Calculations of Absolute Binding Free Energies. Journal of Chemical Theory and Computation, 2011, 7, 2224-2232.	2.3	18
30	Molecular Mimicry and Ligand Recognition in Binding and Catalysis by the Histone Demethylase LSD1-CoREST Complex. Structure, 2011, 19, 212-220.	1.6	85
31	Conformational properties of glucose-based disaccharides investigated using molecular dynamics simulations with local elevation umbrella sampling. Carbohydrate Research, 2010, 345, 1781-1801.	1.1	125
32	How Can Hydrophobic Association Be Enthalpy Driven?. Journal of Chemical Theory and Computation, 2010, 6, 2866-2871.	2.3	205
33	Water in Cavityâ^'Ligand Recognition. Journal of the American Chemical Society, 2010, 132, 12091-12097.	6.6	236
34	Multiple pathways guide oxygen diffusion into flavoenzyme active sites. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 10603-10608.	3.3	157
35	The oxygen-binding vs. oxygen-consuming paradigm in biocatalysis: structural biology and biomolecular simulation. Current Opinion in Structural Biology, 2009, 19, 672-679.	2.6	31
36	Absolute Single-Molecule Entropies from Quasi-Harmonic Analysis of Microsecond Molecular Dynamics: Correction Terms and Convergence Properties. Journal of Chemical Theory and Computation, 2009, 5, 3150-3160.	2.3	75

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37	Independent-Trajectories Thermodynamic-Integration Free-Energy Changes for Biomolecular Systems: Determinants of H5N1 Avian Influenza Virus Neuraminidase Inhibition by Peramivir. Journal of Chemical Theory and Computation, 2009, 5, 1106-1116.	2.3	87
38	On using a too large integration time step in molecular dynamics simulations of coarse-grained molecular models. Physical Chemistry Chemical Physics, 2009, 11, 1934-41.	1.3	76
39	An improved relaxed complex scheme for receptor flexibility in computer-aided drug design. Journal of Computer-Aided Molecular Design, 2008, 22, 693-705.	1.3	283
40	Exploring the Conserved Water Site and Hydration of a Coiledâ€Coil Trimerisation Motif: A MD Simulation Study. ChemBioChem, 2008, 9, 1749-1756.	1.3	7
41	(Thermo)dynamic Role of Receptor Flexibility, Entropy, and Motional Correlation in Proteinâ€“Ligand Binding. ChemPhysChem, 2008, 9, 983-988.	1.0	39
42	Hotâ€spot residues at the E9/Im9 interface help binding via different mechanisms. Biopolymers, 2008, 89, 916-920.	1.2	3
43	Novel Druggable Hot Spots in Avian Influenza Neuraminidase H5N1 Revealed by Computational Solvent Mapping of a Reduced and Representative Receptor Ensemble. Chemical Biology and Drug Design, 2008, 71, 106-116.	1.5	97
44	Water-Membrane Partition Thermodynamics of an Amphiphilic Lipopeptide: An Enthalpy-Driven Hydrophobic Effect. Biophysical Journal, 2008, 95, 3269-3277.	0.2	33
45	E9-Im9 Colicin DNaseâ˜Immunity Protein Biomolecular Association in Water: A Multiple-Copy and Accelerated Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2008, 112, 16802-16814.	1.2	9
46	Entropic contributions and the influence of the hydrophobic environment in promiscuous proteinâ€“protein association. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 7456-7461.	3.3	69
47	Dynamics, Hydration, and Motional Averaging of a Loop-Gated Artificial Protein Cavity:â€‰ The W191G Mutant of Cytochrome c Peroxidase in Water as Revealed by Molecular Dynamics Simulations. Biochemistry, 2007, 46, 10629-10642.	1.2	45
48	Comparison of Thermodynamic Properties of Coarse-Grained and Atomic-Level Simulation Models. ChemPhysChem, 2007, 8, 452-461.	1.0	102
49	Configurational entropy elucidates the role of salt-bridge networks in protein thermostability. Protein Science, 2007, 16, 1349-1359.	3.1	99
50	Comparison of Atomic-Level and Coarse-Grained Models for Liquid Hydrocarbons from Molecular Dynamics Configurational Entropy Estimates. Journal of Physical Chemistry B, 2006, 110, 8464-8473.	1.2	60
51	Configurational Entropy Change of Netropsin and Distamycin upon DNA Minor-Groove Binding. Biophysical Journal, 2006, 91, 1460-1470.	0.2	45
52	Conformational and Dynamical Properties of Disaccharides in Water: a Molecular Dynamics Study. Biophysical Journal, 2006, 90, 4337-4344.	0.2	97
53	Configurational Entropies of Lipids in Pure and Mixed Bilayers from Atomic-Level and Coarse-Grained Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 15602-15614.	1.2	58
54	Biomolecular Modeling: Goals, Problems, Perspectives. Angewandte Chemie - International Edition, 2006, 45, 4064-4092.	7.2	503

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55	The GROMOS software for biomolecular simulation: GROMOS05. Journal of Computational Chemistry, 2005, 26, 1719-1751.	1.5	592
56	Principles of carbopeptoid folding: a molecular dynamics simulation study. Journal of Peptide Science, 2005, 11, 74-84.	0.8	19
57	Carbopeptoid Folding: Effects of Stereochemistry, Chain Length, and Solvent. Angewandte Chemie - International Edition, 2004, 43, 4055-4059.	7.2	24
58	-Peptides with Different Secondary-Structure Preferences: How Different Are Their Conformational Spaces?. Helvetica Chimica Acta, 2002, 85, 3872-3882.	1.0	23