Rebecca C Wade

List of Publications by Citations

274 papers	12,958 citations	65 h-index	102 g-index
316 ext. papers	14,585 ext. citations	6.5 avg, IF	6.45 L-index

#	Paper	IF	Citations
274	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program. *Computer Physics Communications*, **1995**, 91, 57-95	4.2	567
273	New hydrogen-bond potentials for use in determining energetically favorable binding sites on molecules of known structure. *Journal of Medicinal Chemistry*, **1989**, 32, 1083-94	8.3	333
272	How do substrates enter and products exit the buried active site of cytochrome P450cam? 1. Random expulsion molecular dynamics investigation of ligand access channels and mechanisms. *Journal of Molecular Biology*, **2000**, 303, 797-811	6.5	279
271	The ins and outs of cytochrome P450s. *Biochimica Et Biophysica Acta - General Subjects*, **2007**, 1770, 390-401	4	268
270	Simulation of the diffusional association of barnase and barstar. *Biophysical Journal*, **1997**, 72, 1917-29	2.9	253
269	Prediction of drug binding affinities by comparative binding energy analysis. *Journal of Medicinal Chemistry*, **1995**, 38, 2681-91	8.3	239
268	Improving the Continuum Dielectric Approach to Calculating pKas of Ionizable Groups in Proteins. *The Journal of Physical Chemistry*, **1996**, 100, 17373-17387		227
267	Crucial HSP70 co-chaperone complex unlocks metazoan protein disaggregation. *Nature*, **2015**, 524, 247-51	50.4	224
266	Redesigning dehalogenase access tunnels as a strategy for degrading an anthropogenic substrate. *Nature Chemical Biology*, **2009**, 5, 727-33	11.7	207
265	Protein-protein association: investigation of factors influencing association rates by brownian dynamics simulations. *Journal of Molecular Biology*, **2001**, 306, 1139-55	6.5	197
264	Further development of hydrogen bond functions for use in determining energetically favorable binding sites on molecules of known structure. 1. Ligand probe groups with the ability to form two hydrogen bonds. *Journal of Medicinal Chemistry*, **1993**, 36, 140-7	8.3	196
263	Further development of hydrogen bond functions for use in determining energetically favorable binding sites on molecules of known structure. 2. Ligand probe groups with the ability to form more than two hydrogen bonds. *Journal of Medicinal Chemistry*, **1993**, 36, 148-56	8.3	178
262	Biomolecular diffusional association. *Current Opinion in Structural Biology*, **2002**, 12, 204-13	8.1	171
261	Electrostatic steering and ionic tethering in enzyme-ligand binding: insights from simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **1998**, 95, 5942-9	11.5	169
260	Computer simulation of protein-protein association kinetics: acetylcholinesterase-fasciculin. *Journal of Molecular Biology*, **1999**, 291, 149-62	6.5	164
259	Comparison of the dynamics of substrate access channels in three cytochrome P450s reveals different opening mechanisms and a novel functional role for a buried arginine. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 5361-6	11.5	160
258	Allostery in Its Many Disguises: From Theory to Applications. *Structure*, **2019**, 27, 566-578	5.2	158

257	Protein Binding Pocket Dynamics. *Accounts of Chemical Research*, **2016**, 49, 809-15	24.3	156
256	Effective Charges for Macromolecules in Solvent. *The Journal of Physical Chemistry*, **1996**, 100, 3868-3878		152
255	Brownian dynamics simulation of protein-protein diffusional encounter. *Methods*, **1998**, 14, 329-41	4.6	151
254	A survey of active site access channels in cytochromes P450. *Journal of Inorganic Biochemistry*, **2004**, 98, 1175-82	4.2	146
253	Molecular docking using surface complementarity. *Proteins: Structure, Function and Bioinformatics*, **1996**, 25, 120-129	4.2	139
252	How do substrates enter and products exit the buried active site of cytochrome P450cam? 2. Steered molecular dynamics and adiabatic mapping of substrate pathways. *Journal of Molecular Biology*, **2000**, 303, 813-30	6.5	135
251	Computational approaches to identifying and characterizing protein binding sites for ligand design. *Journal of Molecular Recognition*, **2010**, 23, 209-19	2.6	130
250	Structure and dynamics of the membrane-bound cytochrome P450 2C9. *PLoS Computational Biology*, **2011**, 7, e1002152	5	121
249	Do mammalian cytochrome P450s show multiple ligand access pathways and ligand channelling?. *EMBO Reports*, **2005**, 6, 584-9	6.5	114
248	Kinetics for Drug Discovery: an industry-driven effort to target drug residence time. *Drug Discovery Today*, **2017**, 22, 896-911	8.8	113
247	Docking of ubiquitin to gold nanoparticles. *ACS Nano*, **2012**, 6, 9863-78	16.7	112
246	Diffusional encounter of barnase and barstar. *Biophysical Journal*, **2006**, 90, 1913-24	2.9	112
245	Modeling and simulation of protein-surface interactions: achievements and challenges. *Quarterly Reviews of Biophysics*, **2016**, 49, e4	7	112
244	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 323-48	4.2	111
243	Comparative kinetic analysis of FLP and cre recombinases: mathematical models for DNA binding and recombination. *Journal of Molecular Biology*, **1998**, 284, 363-84	6.5	108
242	Visualization of macromolecular structures. *Nature Methods*, **2010**, 7, S42-55	21.6	107
241	A tightly regulated molecular toggle controls AAA+ disaggregase. *Nature Structural and Molecular Biology*, **2012**, 19, 1338-46	17.6	102
240	Protein conformational flexibility modulates kinetics and thermodynamics of drug binding. *Nature Communications*, **2017**, 8, 2276	17.4	101

239	Blue copper proteins: a comparative analysis of their molecular interaction properties. *Protein Science*, **2000**, 9, 1439-54	6.3	96
238	Improving macromolecular electrostatics calculations. *Protein Engineering, Design and Selection*, **1999**, 12, 657-62	1.9	96
237	Estimation of Drug-Target Residence Times by Random Acceleration Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2018**, 14, 3859-3869	6.4	95
236	Theoretical investigation of the dynamics of the active site lid in Rhizomucor miehei lipase. *Biophysical Journal*, **1996**, 71, 119-29	2.9	93
235	Exceptionally stable salt bridges in cytochrome P450cam have functional roles. *Biochemistry*, **1997**, 36, 5402-17	3.2	91
234	Thermodynamics of water mediating protein-ligand interactions in cytochrome P450cam: a molecular dynamics study. *Biophysical Journal*, **1995**, 69, 810-24	2.9	88
233	Importance of explicit salt ions for protein stability in molecular dynamics simulation. *Biophysical Journal*, **1998**, 74, 2906-11	2.9	87
232	Gating of the active site of triose phosphate isomerase: Brownian dynamics simulations of flexible peptide loops in the enzyme. *Biophysical Journal*, **1993**, 64, 9-15	2.9	87
231	Comparative binding energy (COMBINE) analysis of influenza neuraminidase-inhibitor complexes. *Journal of Medicinal Chemistry*, **2001**, 44, 961-71	8.3	86
230	Global profiling of SRP interaction with nascent polypeptides. *Nature*, **2016**, 536, 219-23	50.4	85
229	Computational Alchemy To Calculate Absolute Protein Ligand Binding Free Energy. *Journal of the American Chemical Society*, **1998**, 120, 2710-2713	16.4	84
228	L-Alanyl-L-alanine in the zwitterionic state: structures determined in the presence of explicit water molecules and with continuum models using density functional theory. *Chemical Physics*, **1999**, 240, 63-77	2.3	83
227	Docking of Glycosaminoglycans to Heparin-Binding Proteins: Validation for aFGF, bFGF, and Antithrombin and Application to IL-8. *Journal of the American Chemical Society*, **1999**, 121, 3004-3013	16.4	80
226	New approaches for computing ligand-receptor binding kinetics. *Current Opinion in Structural Biology*, **2018**, 49, 1-10	8.1	80
225	A comparison of aqueous solvent models used in the calculation of the Raman and ROA spectra of l-alanine. *Chemical Physics*, **2001**, 265, 125-151	2.3	79
224	Targeting protein dynamics in drug design. *Journal of Cheminformatics*, **2013**, 5,	8.6	78
223	Brownian dynamics simulation of protein solutions: structural and dynamical properties. *Biophysical Journal*, **2010**, 99, 3782-91	2.9	78
222	Correction for Cardinale et al., Protein-protein interface-binding peptides inhibit the cancer therapy target human thymidylate synthase. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 16133-16133	11.5	78

221	Electrostatic analysis and Brownian dynamics simulation of the association of plastocyanin and cytochrome f. *Biophysical Journal*, **2001**, 81, 3090-104	2.9	77
220	Classification of protein sequences by homology modeling and quantitative analysis of electrostatic similarity. *Proteins: Structure, Function and Bioinformatics*, **1999**, 37, 379-87	4.2	76
219	Pathways and mechanisms for product release in the engineered haloalkane dehalogenases explored using classical and random acceleration molecular dynamics simulations. *Journal of Molecular Biology*, **2009**, 392, 1339-56	6.5	75
218	webPIPSA: a web server for the comparison of protein interaction properties. *Nucleic Acids Research*, **2008**, 36, W276-80	20.1	73
217	How optimal are the binding energetics of barnase and barstar?. *Biophysical Journal*, **2004**, 87, 1618-30	2.9	73
216	On the protein-protein diffusional encounter complex. *Journal of Molecular Recognition*, **1999**, 12, 226-34	1.6	73
215	FluR and structure-based drug design. *Structure*, **1997**, 5, 1139-45	5.2	72
214	Structure and function of the hetero-oligomeric cysteine synthase complex in plants. *Journal of Biological Chemistry*, **2010**, 285, 32810-32817	5.4	71
213	Use of vibrational spectroscopy to study protein and DNA structure, hydration, and binding of biomolecules: A combined theoretical and experimental approach. *International Journal of Quantum Chemistry*, **2006**, 106, 1160-1198	2.1	70
212	A molecular dynamics study of thermodynamic and structural aspects of the hydration of cavities in proteins. *Biopolymers*, **1991**, 31, 919-31	2.2	67
211	Protein-protein interface-binding peptides inhibit the cancer therapy target human thymidylate synthase. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, E542-9	11.5	66
210	A mechanistic model of the cysteine synthase complex. *Journal of Molecular Biology*, **2009**, 386, 37-59	6.5	66
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206	Molecular docking using surface complementarity. *Proteins: Structure, Function and Bioinformatics*, **1996**, 25, 120-9	4.2	61
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204	The shape of protein crowders is a major determinant of protein diffusion. *Biophysical Journal*, **2013**, 104, 1576-84	2.9	58

203	Quantitative analysis of substrate specificity of haloalkane dehalogenase LinB from Sphingomonas paucimobilis UT26. *Biochemistry*, **2005**, 44, 3390-401	3.2	58
202	Heterodimer formation of wild-type and amyotrophic lateral sclerosis-causing mutant Cu/Zn-superoxide dismutase induces toxicity independent of protein aggregation. *Human Molecular Genetics*, **2008**, 17, 1373-85	5.6	57
201	Conformational diversity and ligand tunnels of mammalian cytochrome P450s. *Biotechnology and Applied Biochemistry*, **2013**, 60, 134-45	2.8	55
200	Biochemical network-based drug-target prediction. *Current Opinion in Biotechnology*, **2010**, 21, 511-6	11.4	55
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198	Rational modification of human synovial fluid phospholipase A2 inhibitors. *Journal of Medicinal Chemistry*, **1994**, 37, 337-41	8.3	54
197	pKa calculations for class A beta-lactamases: methodological and mechanistic implications. *Biophysical Journal*, **1997**, 73, 2416-26	2.9	53
196	Improved binding of cytochrome P450cam substrate analogues designed to fill extra space in the substrate binding pocket. *Biochemistry*, **1996**, 35, 1485-99	3.2	53
195	Atomic detail brownian dynamics simulations of concentrated protein solutions with a mean field treatment of hydrodynamic interactions. *Journal of Physical Chemistry B*, **2012**, 116, 8523-33	3.4	52
194	TRAPP: a tool for analysis of transient binding pockets in proteins. *Journal of Chemical Information and Modeling*, **2013**, 53, 1235-52	6.1	52
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192	Towards molecular dynamics simulation of large proteins with a hydration shell at constant pressure. *Biophysical Chemistry*, **1999**, 78, 157-82	3.5	52
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185	SDA 7: A modular and parallel implementation of the simulation of diffusional association software. *Journal of Computational Chemistry*, **2015**, 36, 1631-45	3.5	46
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178	Evolution of an intricate J-protein network driving protein disaggregation in eukaryotes. *ELife*, **2017**, 6,	8.9	41
177	Substrate Access to Cytochrome P450cam: A Comparison of a Thermal Motion Pathway Analysis with Molecular Dynamics Simulation Data. *Journal of Molecular Modeling*, **1997**, 3, 369-374	2	40
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159	Free energies of hydration from thermodynamic integration: Comparison of molecular mechanics force fields and evaluation of calculation accuracy. *Journal of Computational Chemistry*, **1997**, 18, 449-462	3.5	32
158	Structural Basis for Conserved Regulation and Adaptation of the Signal Recognition Particle Targeting Complex. *Journal of Molecular Biology*, **2016**, 428, 2880-97	6.5	32
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148	Comparison of the binding and reactivity of plant and mammalian peroxidases to indole derivatives by computational docking. *Biochemistry*, **2006**, 45, 2940-50	3.2	28
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138	Hydration of cavities in proteins: a molecular dynamics approach. *Journal of the American Chemical Society*, **1990**, 112, 7057-7059	16.4	26
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