Rebecca C Wade

List of Publications by Year in Descending Order

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	The binding of heparin to spike glycoprotein inhibits SARS-CoV-2 infection by three mechanisms.. *Journal of Biological Chemistry*, **2021**, 101507	5.4	9
273	A Blueprint for High Affinity SARS-CoV-2 Mpro Inhibitors from Activity-Based Compound Library Screening Guided by Analysis of Protein Dynamics. *ACS Pharmacology and Translational Science*, **2021**, 4, 1079-1095	5.9	15
272	Brownian Dynamics Simulations of Proteins in the Presence of Surfaces: Long-Range Electrostatics and Mean-Field Hydrodynamics. *Journal of Chemical Theory and Computation*, **2021**, 17, 3510-3524	6.4	1
271	Line-FRAP, A Versatile Method to Measure Diffusion Rates In Vitro and In Vivo. *Journal of Molecular Biology*, **2021**, 433, 166898	6.5	2
270	Structure-kinetic relationship reveals the mechanism of selectivity of FAK inhibitors over PYK2. *Cell Chemical Biology*, **2021**, 28, 686-698.e7	8.2	13
269	Simulation of the Positive Inotropic Peptide S100A1ct in Aqueous Environment by Gaussian Accelerated Molecular Dynamics. *Journal of Physical Chemistry B*, **2021**, 125, 4654-4666	3.4	0
268	A Bittersweet Computational Journey among Glycosaminoglycans. *Biomolecules*, **2021**, 11,	5.9	5
267	Ligand unbinding mechanisms and kinetics for T4 lysozyme mutants from RAMD simulations. *Current Research in Structural Biology*, **2021**, 3, 106-111	2.8	5
266	An electron transfer competent structural ensemble of membrane-bound cytochrome P450 1A1 and cytochrome P450 oxidoreductase. *Communications Biology*, **2021**, 4, 55	6.7	10
265	A Protocol to Use Comparative Binding Energy Analysis to Estimate Drug-Target Residence Time. *Methods in Molecular Biology*, **2021**, 2266, 171-186	1.4	1
264	Putative second hit rare genetic variants in families with seemingly GBA-associated Parkinson's disease. *Npj Genomic Medicine*, **2021**, 6, 2	6.2	1
263	Prediction of the Drug-Target Binding Kinetics for Flexible Proteins by Comparative Binding Energy Analysis. *Journal of Chemical Information and Modeling*, **2021**, 61, 3708-3721	6.1	1
262	G Protein-Coupled Receptor-Ligand Dissociation Rates and Mechanisms from RAMD Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 6610-6623	6.4	1
261	DNA sequence-dependent positioning of the linker histone in a nucleosome: A single-pair FRET study. *Biophysical Journal*, **2021**, 120, 3747-3763	2.9	1
260	Contact Map Fingerprints of Protein-Ligand Unbinding Trajectories Reveal Mechanisms Determining Residence Times Computed from Scaled Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2021**, 17, 6522-6535	6.4	1
259	Structural characterization of an Arf dimer interface: molecular mechanism of Arf-dependent membrane scission. *FEBS Letters*, **2020**, 594, 2240-2253	3.8	3
258	Myotubularin-related protein 7 activates peroxisome proliferator-activated receptor-gamma. *Oncogenesis*, **2020**, 9, 59	6.6	1

257	Computation of FRAP recovery times for linker histone - chromatin binding on the basis of Brownian dynamics simulations. *Biochimica Et Biophysica Acta - General Subjects*, **2020**, 1864, 129653	4	1
256	A function of profilin in force generation during malaria parasite motility that is independent of actin binding. *Journal of Cell Science*, **2020**, 134,	5.3	4
255	Druggability Assessment in TRAPP Using Machine Learning Approaches. *Journal of Chemical Information and Modeling*, **2020**, 60, 1685-1699	6.1	14
254	Chromatosome Structure and Dynamics from Molecular Simulations. *Annual Review of Physical Chemistry*, **2020**, 71, 101-119	15.7	15
253	The Effect of Force-Field Parameters on Cytochrome P450-Membrane Interactions: Structure and Dynamics. *Scientific Reports*, **2020**, 10, 7284	4.9	14
252	RASPD+: Fast Protein-Ligand Binding Free Energy Prediction Using Simplified Physicochemical Features. *Frontiers in Molecular Biosciences*, **2020**, 7, 601065	5.6	5
251	A workflow for exploring ligand dissociation from a macromolecule: Efficient random acceleration molecular dynamics simulation and interaction fingerprint analysis of ligand trajectories. *Journal of Chemical Physics*, **2020**, 153, 125102	3.9	17
250	Recent progress in molecular simulation methods for drug binding kinetics. *Current Opinion in Structural Biology*, **2020**, 64, 126-133	8.1	20
249	Differing Membrane Interactions of Two Highly Similar Drug-Metabolizing Cytochrome P450 Isoforms: CYP 2C9 and CYP 2C19. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	6
248	Influence of Transmembrane Helix Mutations on Cytochrome P450-Membrane Interactions and Function. *Biophysical Journal*, **2019**, 116, 419-432	2.9	13
247	Machine Learning Analysis of RAMD Trajectories to Decipher Molecular Determinants of Drug-Target Residence Times. *Frontiers in Molecular Biosciences*, **2019**, 6, 36	5.6	17
246	Accelerating Drug Discovery Efforts for Trypanosomatidic Infections Using an Integrated Transnational Academic Drug Discovery Platform. *SLAS Discovery*, **2019**, 24, 346-361	3.4	9
245	Allostery in Its Many Disguises: From Theory to Applications. *Structure*, **2019**, 27, 566-578	5.2	158
244	KBbox: A Toolbox of Computational Methods for Studying the Kinetics of Molecular Binding. *Journal of Chemical Information and Modeling*, **2019**, 59, 3630-3634	6.1	7
243	Regulation of adenylyl cyclase 5 in striatal neurons confers the ability to detect coincident neuromodulatory signals. *PLoS Computational Biology*, **2019**, 15, e1007382	5	9
242	A Multi-resolution Approach to the Simulation of Protein Complexes in a Membrane Bilayer **2019**, 505-514		
241	A genetic screen pinpoints ribonucleotide reductase residues that sustain dNTP homeostasis and specifies a highly mutagenic type of dNTP imbalance. *Nucleic Acids Research*, **2019**, 47, 237-252	20.1	10
240	Impact of carbonylation on glutathione peroxidase-1 activity in human hyperglycemic endothelial cells. *Redox Biology*, **2018**, 16, 113-122	11.3	19

239	Halogen-Aromatic Interactions Modulate Inhibitor Residence Times. *Angewandte Chemie - International Edition*, **2018**, 57, 7220-7224	16.4	31
238	Halogenaromatische Wechselwirkungen modulieren die Verweilzeit von Inhibitoren. *Angewandte Chemie*, **2018**, 130, 7338-7343	3.6	1
237	Inter-subunit interactions drive divergent dynamics in mammalian and Plasmodium actin filaments. *PLoS Biology*, **2018**, 16, e2005345	9.7	26
236	New approaches for computing ligand-receptor binding kinetics. *Current Opinion in Structural Biology*, **2018**, 49, 1-10	8.1	80
235	Prediction of Drug-Target Binding Kinetics by Comparative Binding Energy Analysis. *ACS Medicinal Chemistry Letters*, **2018**, 9, 1134-1139	4.3	23
234	The trypanocidal benzoxaborole AN7973 inhibits trypanosome mRNA processing. *PLoS Pathogens*, **2018**, 14, e1007315	7.6	30
233	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
232	Dependence of Chromatosome Structure on Linker Histone Sequence and Posttranslational Modification. *Biophysical Journal*, **2018**, 114, 2363-2375	2.9	22
231	Toward an Ensemble View of Chromatosome Structure: A Paradigm Shift from One to Many. *Structure*, **2018**, 26, 1050-1057	5.2	22
230	Kinetics for Drug Discovery: an industry-driven effort to target drug residence time. *Drug Discovery Today*, **2017**, 22, 896-911	8.8	113
229	Evolution of an intricate J-protein network driving protein disaggregation in eukaryotes. *ELife*, **2017**, 6,	8.9	41
228	Exploiting the 2-Amino-1,3,4-thiadiazole Scaffold To Inhibit Pteridine Reductase in Support of Early-Stage Drug Discovery. *ACS Omega*, **2017**, 2, 5666-5683	3.9	17
227	Comparative mapping of on-targets and off-targets for the discovery of anti-trypanosomatid folate pathway inhibitors. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 3215-3230	4	8
226	Application of a simple quantum chemical approach to ligand fragment scoring for Trypanosoma brucei pteridine reductase 1 inhibition. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 715-728	4.2	6
225	A novel homozygous ARL13B variant in patients with Joubert syndrome impairs its guanine nucleotide-exchange factor activity. *European Journal of Human Genetics*, **2017**, 25, 1324-1334	5.3	4
224	TRAPP webserver: predicting protein binding site flexibility and detecting transient binding pockets. *Nucleic Acids Research*, **2017**, 45, W325-W330	20.1	25
223	Protein conformational flexibility modulates kinetics and thermodynamics of drug binding. *Nature Communications*, **2017**, 8, 2276	17.4	101
222	Chroman-4-One Derivatives Targeting Pteridine Reductase 1 and Showing Anti-Parasitic Activity. *Molecules*, **2017**, 22,	4.8	25

221	A unique profilin-actin interface is important for malaria parasite motility. *PLoS Pathogens*, **2017**, 13, e1006412	7.6	34
220	Ligand tunnels in T. brucei and human CYP51: Insights for parasite-specific drug design. *Biochimica Et Biophysica Acta - General Subjects*, **2016**, 1860, 67-78	4	18
219	Profiling of Flavonol Derivatives for the Development of Antitrypanosomatidic Drugs. *Journal of Medicinal Chemistry*, **2016**, 59, 7598-616	8.3	30
218	The HMGB1 protein induces a metabolic type of tumour cell death by blocking aerobic respiration. *Nature Communications*, **2016**, 7, 10764	17.4	30
217	Conformational selection and dynamic adaptation upon linker histone binding to the nucleosome. *Nucleic Acids Research*, **2016**, 44, 6599-613	20.1	27
216	Identification of an Electrostatic Ruler Motif for Sequence-Specific Binding of Collagenase to Collagen. *Journal of Physical Chemistry B*, **2016**, 120, 8580-9	3.4	3
215	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. *Journal of Cheminformatics*, **2016**, 8, 18	8.6	
214	ProSAT+: visualizing sequence annotations on 3D structure. *Protein Engineering, Design and Selection*, **2016**, 29, 281-4	1.9	3
213	Homozygous missense mutation in the LMAN2L gene segregates with intellectual disability in a large consanguineous Pakistani family. *Journal of Medical Genetics*, **2016**, 53, 138-44	5.8	10
212	Dynathor: Dynamics of the Complex of Cytochrome P450 and Cytochrome P450 Reductase in a Phospholipid Bilayer **2016**, 255-264		2
211	Human DPP III Keap1 Interactions: A Combined Experimental And Computational Study. *Croatica Chemica Acta*, **2016**, 89,	0.8	4
210	Perturbation Approaches for Exploring Protein Binding Site Flexibility to Predict Transient Binding Pockets. *Journal of Chemical Theory and Computation*, **2016**, 12, 4100-13	6.4	20
209	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
208	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
207	Three steps to gold: mechanism of protein adsorption revealed by Brownian and molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2016**, 18, 10191-200	3.6	22
206	Modeling and simulation of protein-surface interactions: achievements and challenges. *Quarterly Reviews of Biophysics*, **2016**, 49, e4	7	112
205	Protein Binding Pocket Dynamics. *Accounts of Chemical Research*, **2016**, 49, 809-15	24.3	156
204	Comparative electrostatic analysis of adenylyl cyclase for isoform dependent regulation properties. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 1844-1858	4.2	4

203	An Efficient Low Storage and Memory Treatment of Gridded Interaction Fields for Simulations of Macromolecular Association. *Journal of Chemical Theory and Computation*, **2016**, 12, 4563-77	6.4	1
202	Global profiling of SRP interaction with nascent polypeptides. *Nature*, **2016**, 536, 219-23	50.4	85
201	Dynamics of CYP51: implications for function and inhibitor design. *Journal of Molecular Recognition*, **2015**, 28, 59-73	2.6	27
200	Crucial HSP70 co-chaperone complex unlocks metazoan protein disaggregation. *Nature*, **2015**, 524, 247-51	50.4	224
199	Kar1 binding to Sfi1 C-terminal regions anchors the SPB bridge to the nuclear envelope. *Journal of Cell Biology*, **2015**, 209, 843-61	7.3	19
198	Hotspots in an obligate homodimeric anticancer target. Structural and functional effects of interfacial mutations in human thymidylate synthase. *Journal of Medicinal Chemistry*, **2015**, 58, 3572-81	8.3	18
197	When the Label Matters: Adsorption of Labeled and Unlabeled Proteins on Charged Surfaces. *Nano Letters*, **2015**, 15, 7508-13	11.5	17
196	Molecular simulations reveal that the long range fluctuations of human DPP III change upon ligand binding. *Molecular BioSystems*, **2015**, 11, 3068-80		16
195	Computational Approaches for Studying Drug Binding Kinetics. *Methods and Principles in Medicinal Chemistry*, **2015**, 211-235	0.4	4
194	On the application of the MARTINI coarse-grained model to immersion of a protein in a phospholipid bilayer. *Journal of Chemical Physics*, **2015**, 143, 243139	3.9	15
193	webSDA: a web server to simulate macromolecular diffusional association. *Nucleic Acids Research*, **2015**, 43, W220-4	20.1	9
192	A multiscale approach to simulating the conformational properties of unbound multi-C□□zinc finger proteins. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 1604-15	4.2	1
191	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
190	LigDig: a web server for querying ligand-protein interactions. *Bioinformatics*, **2015**, 31, 1147-9	7.2	11
189	Conservation and Role of Electrostatics in Thymidylate Synthase. *Scientific Reports*, **2015**, 5, 17356	4.9	5
188	Long range Debye-H□kel correction for computation of grid-based electrostatic forces between biomacromolecules. *BMC Biophysics*, **2014**, 7, 4	0	6
187	Structure and Dynamics of Human Drug-Metabolizing Cytochrome P450 Enzymes. *Methods and Principles in Medicinal Chemistry*, **2014**, 75-102	0.4	3
186	On calculation of the electrostatic potential of a phosphatidylinositol phosphate-containing phosphatidylcholine lipid membrane accounting for membrane dynamics. *PLoS ONE*, **2014**, 9, e104778	3.7	3

185	Targeting protein dynamics in drug design. *Journal of Cheminformatics*, **2013**, 5,	8.6	78
184	Dynamic enzyme docking to the ribosome coordinates N-terminal processing with polypeptide folding. *Nature Structural and Molecular Biology*, **2013**, 20, 843-50	17.6	49
183	Regulation of the activity of lactate dehydrogenases from four lactic acid bacteria. *Journal of Biological Chemistry*, **2013**, 288, 21295-21306	5.4	29
182	Ligand-based discovery of N-(1,3-dioxo-1H,3H-benzo[de]isochromen-5-yl)-carboxamide and sulfonamide derivatives as thymidylate synthase A inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 663-8	2.9	8
181	GTP regulates the microtubule nucleation activity of γ-tubulin. *Nature Cell Biology*, **2013**, 15, 1317-27	23.4	19
180	Brownian dynamics simulation of protein diffusion in crowded environments **2013**,		1
179	TRAPP: a tool for analysis of transient binding pockets in proteins. *Journal of Chemical Information and Modeling*, **2013**, 53, 1235-52	6.1	52
178	Conformational diversity and ligand tunnels of mammalian cytochrome P450s. *Biotechnology and Applied Biochemistry*, **2013**, 60, 134-45	2.8	55
177	The shape of protein crowders is a major determinant of protein diffusion. *Biophysical Journal*, **2013**, 104, 1576-84	2.9	58
176	Organism-adapted specificity of the allosteric regulation of pyruvate kinase in lactic acid bacteria. *PLoS Computational Biology*, **2013**, 9, e1003159	5	11
175	Translational repression of thymidylate synthase by targeting its mRNA. *Nucleic Acids Research*, **2013**, 41, 4159-70	20.1	8
174	Allosterically gated enzyme dynamics in the cysteine synthase complex regulate cysteine biosynthesis in Arabidopsis thaliana. *Structure*, **2012**, 20, 292-302	5.2	24
173	Docking of ubiquitin to gold nanoparticles. *ACS Nano*, **2012**, 6, 9863-78	16.7	112
172	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
171	A tightly regulated molecular toggle controls AAA+ disaggregase. *Nature Structural and Molecular Biology*, **2012**, 19, 1338-46	17.6	102
170	The interaction properties of the human Rab GTPase family--comparative analysis reveals determinants of molecular binding selectivity. *PLoS ONE*, **2012**, 7, e34870	3.7	32
169	A single mutation in a tunnel to the active site changes the mechanism and kinetics of product release in haloalkane dehalogenase LinB. *Journal of Biological Chemistry*, **2012**, 287, 29062-74	5.4	49
168	Multiple, ligand-dependent routes from the active site of cytochrome P450 2C9. *Current Drug Metabolism*, **2012**, 13, 143-54	3.5	28

167	Structure and dynamics of the membrane-bound cytochrome P450 2C9. *PLoS Computational Biology*, **2011**, 7, e1002152	5	121
166	Virtual screening identification of nonfolate compounds, including a CNS drug, as antiparasitic agents inhibiting pteridine reductase. *Journal of Medicinal Chemistry*, **2011**, 54, 211-21	8.3	52
165	Receptor flexibility in small-molecule docking calculations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 298-314	7.9	38
164	Diffusion and association processes in biological systems: theory, computation and experiment. *BMC Biophysics*, **2011**, 4, 2	0	29
163	Diffusion of hydrophobin proteins in solution and interactions with a graphite surface. *BMC Biophysics*, **2011**, 4, 9	0	13
162	The active-inactive transition of human thymidylate synthase: targeted molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2886-99	4.2	13
161	A quantitative, real-time assessment of binding of peptides and proteins to gold surfaces. *Chemistry - A European Journal*, **2011**, 17, 1327-36	4.8	34
160	Structural basis for the varying propensities of different amino acids to adopt the collagen conformation. *Journal of Physical Chemistry B*, **2011**, 115, 2593-607	3.4	18
159	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
158	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
157	On the structure and dynamics of the complex of the nucleosome and the linker histone. *Nucleic Acids Research*, **2011**, 39, 5255-63	20.1	39
156	Visualization of macromolecular structures. *Nature Methods*, **2010**, 7, S42-55	21.6	107
155	Design and characterization of a mutation outside the active site of human thymidylate synthase that affects ligand binding. *Protein Engineering, Design and Selection*, **2010**, 23, 81-9	1.9	5
154	Homodimeric enzymes as drug targets. *Current Medicinal Chemistry*, **2010**, 17, 826-46	4.3	37
153	Brownian dynamics simulation of protein solutions: structural and dynamical properties. *Biophysical Journal*, **2010**, 99, 3782-91	2.9	78
152	ProMetCS: An Atomistic Force Field for Modeling Protein-Metal Surface Interactions in a Continuum Aqueous Solvent. *Journal of Chemical Theory and Computation*, **2010**, 6, 1753-68	6.4	51
151	Structure and function of the hetero-oligomeric cysteine synthase complex in plants. *Journal of Biological Chemistry*, **2010**, 285, 32810-32817	5.4	71
150	Kinetics of Biomacromolecular Complex Formation: Theory and Experiment **2010**, 89-118		

149	Novel approaches for targeting thymidylate synthase to overcome the resistance and toxicity of anticancer drugs. *Journal of Medicinal Chemistry*, **2010**, 53, 6539-49	8.3	38
148	Computational approaches to identifying and characterizing protein binding sites for ligand design. *Journal of Molecular Recognition*, **2010**, 23, 209-19	2.6	130
147	Protein-surface interactions: challenging experiments and computations. *Journal of Molecular Recognition*, **2010**, 23, 259-62	2.6	33
146	Cross-species analysis of the glycolytic pathway by comparison of molecular interaction fields. *Molecular BioSystems*, **2010**, 6, 152-64		13
145	Biochemical network-based drug-target prediction. *Current Opinion in Biotechnology*, **2010**, 21, 511-6	11.4	55
144	Comparative binding energy analysis for binding affinity and target selectivity prediction. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 135-53	4.2	18
143	Redesigning dehalogenase access tunnels as a strategy for degrading an anthropogenic substrate. *Nature Chemical Biology*, **2009**, 5, 727-33	11.7	207
142	A mechanistic model of the cysteine synthase complex. *Journal of Molecular Biology*, **2009**, 386, 37-59	6.5	66
141	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
140	On the contributions of diffusion and thermal activation to electron transfer between Phormidium laminosum plastocyanin and cytochrome f: Brownian dynamics simulations with explicit modeling of nonpolar desolvation interactions and electron transfer events. *Journal of the American Chemical Society*, **2009**, 131, 9230-8	16.4	45
139	Molecular Recognition: Computational Analysis and Modelling **2008**, 1		
138	Mechanism of auxin interaction with Auxin Binding Protein (ABP1): a molecular dynamics simulation study. *Biophysical Journal*, **2008**, 94, 27-37	2.9	42
137	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
136	SYCAMORE--a systems biology computational analysis and modeling research environment. *Bioinformatics*, **2008**, 24, 1463-4	7.2	26
135	webPIPSA: a web server for the comparison of protein interaction properties. *Nucleic Acids Research*, **2008**, 36, W276-80	20.1	73
134	Calculating enzyme kinetic parameters from protein structures. *Biochemical Society Transactions*, **2008**, 36, 51-4	5.1	8
133	Protein-protein docking by simulating the process of association subject to biochemical constraints. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 1955-69	4.2	24
132	On the use of PIPSA to guide target-selective drug design. *ChemMedChem*, **2008**, 3, 413-7	3.7	11

131	Structural and electrostatic properties of ubiquitination and related pathways. *Frontiers in Bioscience - Landmark*, **2007**, 12, 3419-30	2.8	9
130	COMBINE analysis of the specificity of binding of Ras proteins to their effectors. *Proteins: Structure, Function and Bioinformatics*, **2007**, 67, 435-47	4.2	19
129	qPIPSA: relating enzymatic kinetic parameters and interaction fields. *BMC Bioinformatics*, **2007**, 8, 373	3.6	36
128	Bridging from molecular simulation to biochemical networks. *Current Opinion in Structural Biology*, **2007**, 17, 166-72	8.1	39
127	The ins and outs of cytochrome P450s. *Biochimica Et Biophysica Acta - General Subjects*, **2007**, 1770, 390-401	4	268
126	FTIR studies of the redox partner interaction in cytochrome P450: the Pdx-P450cam couple. *Biochimica Et Biophysica Acta - General Subjects*, **2007**, 1770, 420-31	4	15
125	On the Use of Elevated Temperature in Simulations To Study Protein Unfolding Mechanisms. *Journal of Chemical Theory and Computation*, **2007**, 3, 1476-83	6.4	21
124	ProSAT2--Protein Structure Annotation Server. *Nucleic Acids Research*, **2006**, 34, W79-83	20.1	10
123	Diffusional encounter of barnase and barstar. *Biophysical Journal*, **2006**, 90, 1913-24	2.9	112
122	Force Field Effects on a β-Sheet Protein Domain Structure in Thermal Unfolding Simulations. *Journal of Chemical Theory and Computation*, **2006**, 2, 140-8	6.4	23
121	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
120	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
119	Quantitative analysis of substrate specificity of haloalkane dehalogenase LinB from Sphingomonas paucimobilis UT26. *Biochemistry*, **2005**, 44, 3390-401	3.2	58
118	The impact of protein flexibility on protein-protein docking. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 126-33	4.2	35
117	Issues in high-throughput comparative modelling: a case study using the ubiquitin E2 conjugating enzymes. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 367-75	4.2	5
116	Multiple molecular recognition mechanisms. Cytochrome P450--a case study. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2005**, 1754, 239-44	4	28
115	Do mammalian cytochrome P450s show multiple ligand access pathways and ligand channelling?. *EMBO Reports*, **2005**, 6, 584-9	6.5	114
114	Calculation and Application of Molecular Interaction Fields. *Methods and Principles in Medicinal Chemistry*, **2005**, 27-42	0.4	4

113	Determinants of functionality in the ubiquitin conjugating enzyme family. *Structure*, **2004**, 12, 1563-74	5.2	43
112	Computational approaches to structural and functional analysis of plastocyanin and other blue copper proteins. *Cellular and Molecular Life Sciences*, **2004**, 61, 1123-42	10.3	21
111	A survey of active site access channels in cytochromes P450. *Journal of Inorganic Biochemistry*, **2004**, 98, 1175-82	4.2	146
110	Using 3D protein structures to derive 3D-QSARs. *Drug Discovery Today: Technologies*, **2004**, 1, 241-6	7.1	7
109	How optimal are the binding energetics of barnase and barstar?. *Biophysical Journal*, **2004**, 87, 1618-30	2.9	73
108	Comparative structural and energetic analysis of WW domain-peptide interactions. *Journal of Molecular Biology*, **2004**, 344, 865-81	6.5	34
107	Implicit solvent models for flexible protein-protein docking by molecular dynamics simulation. *Proteins: Structure, Function and Bioinformatics*, **2003**, 50, 158-69	4.2	60
106	Comparative binding energy analysis of haloalkane dehalogenase substrates: modelling of enzyme-substrate complexes by molecular docking and quantum mechanical calculations. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 299-311	4.2	18
105	Inhibitor specificity via protein dynamics: insights from the design of antibacterial agents targeted against thymidylate synthase. *Chemistry and Biology*, **2003**, 10, 1183-93		28
104	A new approach to predict the biological activity of molecules based on similarity of their interaction fields and the logP and logD values: application to auxins. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1532-41		11
103	In search of the prototype of nitric oxide synthase. *FEBS Letters*, **2003**, 554, 1-5	3.8	20
102	Concerted simulations reveal how peroxidase compound III formation results in cellular oscillations. *Biophysical Journal*, **2003**, 85, 1421-8	2.9	19
101	MolSurfer: A macromolecular interface navigator. *Nucleic Acids Research*, **2003**, 31, 3349-51	20.1	40
100	ProSAT: functional annotation of protein 3D structures. *Bioinformatics*, **2003**, 19, 1723-5	7.2	12
99	DSMM: a Database of Simulated Molecular Motions. *Nucleic Acids Research*, **2003**, 31, 456-7	20.1	9
98	Biomolecular diffusional association. *Current Opinion in Structural Biology*, **2002**, 12, 204-13	8.1	171
97	Elusive recognition determinants for ubiquitination. *Journal of Molecular Recognition*, **2002**, 15, 3-5	2.6	2
96	Specific and non-specific effects of potassium cations on substrate-protein interactions in cytochromes P450cam and P450lin. *Journal of Inorganic Biochemistry*, **2002**, 91, 597-606	4.2	17

95	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
94	Comparative binding energy (COMBINE) analysis of OppA-peptide complexes to relate structure to binding thermodynamics. *Journal of Medicinal Chemistry*, **2002**, 45, 4828-37	8.3	46
93	Comparative Binding Energy Analysis **2002**, 19-34		2
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