Brian K Shoichet

List of Publications by Year in Descending Order

196 papers	33,713 citations	93 h-index	183 g-index
210 ext. papers	39,288 ext. citations	12.7 avg, IF	7.42 L-index

#	Paper	IF	Citations
196	Structure-Based Design of a Chemical Probe Set for the 5-HT Serotonin Receptor.. *Journal of Medicinal Chemistry*, **2022**,	8.3	3
195	Drug building blocks and libraries at risk in Ukraine. *Science*, **2022**, 376, 929-929	33.3	1
194	Structures of the receptor enable docking for bioactive ligand discovery. *Nature*, **2021**,	50.4	24
193	Structure, function and pharmacology of human itch GPCRs. *Nature*, **2021**, 600, 170-175	50.4	15
192	Colloidal Aggregators in Biochemical SARS-CoV-2 Repurposing Screens. *Journal of Medicinal Chemistry*, **2021**, 64, 17530-17539	8.3	5
191	A practical guide to large-scale docking. *Nature Protocols*, **2021**, 16, 4799-4832	18.8	35
190	Phospholipidosis is a shared mechanism underlying the antiviral activity of many repurposed drugs against SARS-CoV-2 **2021**,		1
189	Fragment binding to the Nsp3 macrodomain of SARS-CoV-2 identified through crystallographic screening and computational docking. *Science Advances*, **2021**, 7,	14.3	41
188	Drug-induced phospholipidosis confounds drug repurposing for SARS-CoV-2. *Science*, **2021**, 373, 541-547	33.3	64
187	Property-Unmatched Decoys in Docking Benchmarks. *Journal of Chemical Information and Modeling*, **2021**, 61, 699-714	6.1	10
186	A Crowding Barrier to Protein Inhibition in Colloidal Aggregates. *Journal of Medicinal Chemistry*, **2021**, 64, 4109-4116	8.3	3
185	Energy penalties enhance flexible receptor docking in a model cavity. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	2
184	Ligand Strain Energy in Large Library Docking. *Journal of Chemical Information and Modeling*, **2021**, 61, 4331-4341	6.1	8
183	Efficient Exploration of Chemical Space with Docking and Deep Learning. *Journal of Chemical Theory and Computation*, **2021**, 17, 7106-7119	6.4	12
182	An allosteric modulator binds to a conformational hub in the adrenergic receptor. *Nature Chemical Biology*, **2020**, 16, 749-755	11.7	16
181	Bacterial metabolism rescues the inhibition of intestinal drug absorption by food and drug additives. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 16009-16018	11.5	15
180	Virtual discovery of melatonin receptor ligands to modulate circadian rhythms. *Nature*, **2020**, 579, 609-614	50.4	88

179	The Global Phosphorylation Landscape of SARS-CoV-2 Infection. *Cell*, **2020**, 182, 685-712.e19	56.2	439
178	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. *Nature*, **2020**, 583, 459-468	50.4	2142
177	Discovery of Lysine-Targeted eIF4E Inhibitors through Covalent Docking. *Journal of the American Chemical Society*, **2020**, 142, 4960-4964	16.4	26
176	Interactions of Oral Molecular Excipients with Breast Cancer Resistance Protein, BCRP. *Molecular Pharmaceutics*, **2020**, 17, 748-756	5.6	12
175	A SARS-CoV-2-Human Protein-Protein Interaction Map Reveals Drug Targets and Potential Drug-Repurposing **2020**,		133
174	Fragment Binding to the Nsp3 Macrodomain of SARS-CoV-2 Identified Through Crystallographic Screening and Computational Docking **2020**,		6
173	Comparative host-coronavirus protein interaction networks reveal pan-viral disease mechanisms. *Science*, **2020**, 370,	33.3	261
172	The activities of drug inactive ingredients on biological targets. *Science*, **2020**, 369, 403-413	33.3	34
171	Differential Roles of Extracellular Histidine Residues of GPR68 for Proton-Sensing and Allosteric Modulation by Divalent Metal Ions. *Biochemistry*, **2020**, 59, 3594-3614	3.2	3
170	Structure of a Hallucinogen-Activated Gq-Coupled 5-HT Serotonin Receptor. *Cell*, **2020**, 182, 1574-1588.e19	56.2	101
169	Structural identification of a hotspot on CFTR for potentiation. *Science*, **2019**, 364, 1184-1188	33.3	96
168	Triggered Release Enhances the Cytotoxicity of Stable Colloidal Drug Aggregates. *ACS Chemical Biology*, **2019**, 14, 1507-1514	4.9	5
167	Colloidal Drug Aggregate Stability in High Serum Conditions and Pharmacokinetic Consequence. *ACS Chemical Biology*, **2019**, 14, 751-757	4.9	16
166	Ultra-large library docking for discovering new chemotypes. *Nature*, **2019**, 566, 224-229	50.4	309
165	Protein Stability Effects in Aggregate-Based Enzyme Inhibition. *Journal of Medicinal Chemistry*, **2019**, 62, 9593-9599	8.3	9
164	GAIN domain-mediated cleavage is required for activation of G protein-coupled receptor 56 (GPR56) by its natural ligands and a small-molecule agonist. *Journal of Biological Chemistry*, **2019**, 294, 19246-19254	5.4	22
163	Structure-based discovery of selective positive allosteric modulators of antagonists for the M muscarinic acetylcholine receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E2419-E2428	11.5	38
162	Structure of the D2 dopamine receptor bound to the atypical antipsychotic drug risperidone. *Nature*, **2018**, 555, 269-273	50.4	243

161	Colloidal aggregation: from screening nuisance to formulation nuance. *Nano Today*, **2018**, 19, 188-200	17.9	44
160	The Psychiatric Cell Map Initiative: A Convergent Systems Biological Approach to Illuminating Key Molecular Pathways in Neuropsychiatric Disorders. *Cell*, **2018**, 174, 505-520	56.2	69
159	Selectivity Challenges in Docking Screens for GPCR Targets and Antitargets. *Journal of Medicinal Chemistry*, **2018**, 61, 6830-6845	8.3	24
158	The Recognition of Unrelated Ligands by Identical Proteins. *ACS Chemical Biology*, **2018**, 13, 2522-2533	4.9	2
157	Structure-inspired design of β-arrestin-biased ligands for aminergic GPCRs. *Nature Chemical Biology* , **2018**, 14, 126-134	11.7	96
156	Structure-guided development of selective M3 muscarinic acetylcholine receptor antagonists. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 12046-12050	11.5	39
155	Far away from the lamppost. *PLoS Biology*, **2018**, 16, e3000067	9.7	10
154	Prediction of enzymatic pathways by integrative pathway mapping. *ELife*, **2018**, 7,	8.9	22
153	Crystal Structure of an LSD-Bound Human Serotonin Receptor. *Cell*, **2017**, 168, 377-389.e12	56.2	214
152	Leveraging Colloidal Aggregation for Drug-Rich Nanoparticle Formulations. *Molecular Pharmaceutics*, **2017**, 14, 1852-1860	5.6	14
151	In silico design of novel probes for the atypical opioid receptor MRGPRX2. *Nature Chemical Biology*, **2017**, 13, 529-536	11.7	158
150	A New Spin on Antibody-Drug Conjugates: Trastuzumab-Fulvestrant Colloidal Drug Aggregates Target HER2-Positive Cells. *ACS Applied Materials & Interfaces*, **2017**, 9, 12195-12202	9.5	18
149	Internal Structure and Preferential Protein Binding of Colloidal Aggregates. *ACS Chemical Biology*, **2017**, 12, 282-290	4.9	19
148	Structure-Based Design and Discovery of New M Receptor Agonists. *Journal of Medicinal Chemistry*, **2017**, 60, 9239-9250	8.3	16
147	Discovery of new GPCR ligands to illuminate new biology. *Nature Chemical Biology*, **2017**, 13, 1143-1151	11.7	52
146	D dopamine receptor high-resolution structures enable the discovery of selective agonists. *Science*, **2017**, 358, 381-386	33.3	128
145	Testing inhomogeneous solvation theory in structure-based ligand discovery. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E6839-E6846	11.5	42
144	Reverse translation of adverse event reports paves the way for de-risking preclinical off-targets. *ELife*, **2017**, 6,	8.9	28

143	Structure-based discovery of opioid analgesics with reduced side effects. *Nature*, **2016**, 537, 185-190	50.4	547
142	Docking Screens for Novel Ligands Conferring New Biology. *Journal of Medicinal Chemistry*, **2016**, 59, 4103-20	8.3	166
141	Stable Colloidal Drug Aggregates Catch and Release Active Enzymes. *ACS Chemical Biology*, **2016**, 11, 992-1000	4.9	23
140	Docking and Linking of Fragments To Discover Jumonji Histone Demethylase Inhibitors. *Journal of Medicinal Chemistry*, **2016**, 59, 1580-98	8.3	40
139	Ligand Similarity Complements Sequence, Physical Interaction, and Co-Expression for Gene Function Prediction. *PLoS ONE*, **2016**, 11, e0160098	3.7	6
138	In Vitro and In Vivo Characterization of the Alkaloid Nuciferine. *PLoS ONE*, **2016**, 11, e0150602	3.7	18
137	Identification of Novel Smoothened Ligands Using Structure-Based Docking. *PLoS ONE*, **2016**, 11, e0160365	3.7	13
136	Hydrogen Bonding of 1,2-Azaborines in the Binding Cavity of T4 Lysozyme Mutants: Structures and Thermodynamics. *Journal of the American Chemical Society*, **2016**, 138, 12021-4	16.4	49
135	Design, Synthesis, and Biological Evaluation of Novel Tetrahydroprotoberberine Derivatives (THPBs) as Selective Adrenoceptor Antagonists. *Journal of Medicinal Chemistry*, **2016**, 59, 9489-9502	8.3	17
134	Virtual Screening for UDP-Galactopyranose Mutase Ligands Identifies a New Class of Antimycobacterial Agents. *ACS Chemical Biology*, **2015**, 10, 2209-18	4.9	28
133	The promise and peril of chemical probes. *Nature Chemical Biology*, **2015**, 11, 536-41	11.7	523
132	Homologous ligands accommodated by discrete conformations of a buried cavity. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 5039-44	11.5	29
131	The Recognition of Identical Ligands by Unrelated Proteins. *ACS Chemical Biology*, **2015**, 10, 2772-84	4.9	52
130	Activity-Independent Discovery of Secondary Metabolites Using Chemical Elicitation and Cheminformatic Inference. *ACS Chemical Biology*, **2015**, 10, 2616-23	4.9	34
129	Small-Molecule Allosteric Modulators of the Protein Kinase PDK1 from Structure-Based Docking. *Journal of Medicinal Chemistry*, **2015**, 58, 8285-8291	8.3	19
128	An Aggregation Advisor for Ligand Discovery. *Journal of Medicinal Chemistry*, **2015**, 58, 7076-87	8.3	258
127	Prediction and validation of enzyme and transporter off-targets for metformin. *Journal of Pharmacokinetics and Pharmacodynamics*, **2015**, 42, 463-75	2.7	32
126	Allosteric ligands for the pharmacologically dark receptors GPR68 and GPR65. *Nature*, **2015**, 527, 477-83	50.4	158

125	One Crystal, Two Temperatures: Cryocooling Penalties Alter Ligand Binding to Transient Protein Sites. *ChemBioChem*, **2015**, 16, 1560-4	3.8	51
124	Colloidal aggregation and the in vitro activity of traditional Chinese medicines. *ACS Chemical Biology*, **2015**, 10, 978-88	4.9	48
123	Large-scale identification and analysis of suppressive drug interactions. *Chemistry and Biology*, **2014** , 21, 541-551		25
122	Incorporation of protein flexibility and conformational energy penalties in docking screens to improve ligand discovery. *Nature Chemistry*, **2014**, 6, 575-83	17.6	90
121	Covalent docking of large libraries for the discovery of chemical probes. *Nature Chemical Biology*, **2014**, 10, 1066-72	11.7	178
120	Colloidal drug formulations can explain "bell-shaped" concentration-response curves. *ACS Chemical Biology*, **2014**, 9, 777-84	4.9	87
119	Actin is required for IFT regulation in Chlamydomonas reinhardtii. *Current Biology*, **2014**, 24, 2025-32	6.3	51
118	Functional annotation and structural characterization of a novel lactonase hydrolyzing D-xylono-1,4-lactone-5-phosphate and L-arabino-1,4-lactone-5-phosphate. *Biochemistry*, **2014**, 53, 4727-38	3.2	8
117	Increasing chemical space coverage by combining empirical and computational fragment screens. *ACS Chemical Biology*, **2014**, 9, 1528-35	4.9	40
116	Blind prediction of charged ligand binding affinities in a model binding site. *Journal of Molecular Biology*, **2013**, 425, 4569-83	6.5	44
115	Chemical informatics uncovers a new role for moexipril as a novel inhibitor of cAMP phosphodiesterase-4 (PDE4). *Biochemical Pharmacology*, **2013**, 85, 1297-305	6	14
114	Assignment of pterin deaminase activity to an enzyme of unknown function guided by homology modeling and docking. *Journal of the American Chemical Society*, **2013**, 135, 795-803	16.4	28
113	A pharmacological organization of G protein-coupled receptors. *Nature Methods*, **2013**, 10, 140-6	21.6	85
112	Colloidal aggregation causes inhibition of G protein-coupled receptors. *Journal of Medicinal Chemistry*, **2013**, 56, 2406-14	8.3	76
111	The impact of introducing a histidine into an apolar cavity site on docking and ligand recognition. *Journal of Medicinal Chemistry*, **2013**, 56, 2874-84	8.3	7
110	Functional annotation and three-dimensional structure of an incorrectly annotated dihydroorotase from cog3964 in the amidohydrolase superfamily. *Biochemistry*, **2013**, 52, 228-38	3.2	8
109	Muscarinic receptors as model targets and antitargets for structure-based ligand discovery. *Molecular Pharmacology*, **2013**, 84, 528-40	4.3	49
108	Roles for ordered and bulk solvent in ligand recognition and docking in two related cavities. *PLoS ONE*, **2013**, 8, e69153	3.7	18

107	Ligand pose and orientational sampling in molecular docking. *PLoS ONE*, **2013**, 8, e75992	3.7	83
106	Identifying mechanism-of-action targets for drugs and probes. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 11178-83	11.5	132
105	Fragment-guided design of subnanomolar β-lactamase inhibitors active in vivo. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 17448-53	11.5	59
104	Structure-based drug screening for G-protein-coupled receptors. *Trends in Pharmacological Sciences* , **2012**, 33, 268-72	13.2	229
103	Directory of useful decoys, enhanced (DUD-E): better ligands and decoys for better benchmarking. *Journal of Medicinal Chemistry*, **2012**, 55, 6582-94	8.3	1022
102	Large-scale prediction and testing of drug activity on side-effect targets. *Nature*, **2012**, 486, 361-7	50.4	623
101	Colloidal aggregation affects the efficacy of anticancer drugs in cell culture. *ACS Chemical Biology*, **2012**, 7, 1429-35	4.9	118
100	Structure-based ligand discovery for the protein-protein interface of chemokine receptor CXCR4. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 5517-22	11.5	123
99	Ligand discovery from a dopamine D3 receptor homology model and crystal structure. *Nature Chemical Biology*, **2011**, 7, 769-78	11.7	250
98	Statistical potential for modeling and ranking of protein-ligand interactions. *Journal of Chemical Information and Modeling*, **2011**, 51, 3078-92	6.1	61
97	Structure-based discovery of prescription drugs that interact with the norepinephrine transporter, NET. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 15810-5	11.5	101
96	The Enzyme Function Initiative. *Biochemistry*, **2011**, 50, 9950-62	3.2	140
95	Rapid behavior-based identification of neuroactive small molecules in the zebrafish. *Nature Chemical Biology*, **2010**, 6, 231-237	11.7	398
94	Design, synthesis, crystal structures, and antimicrobial activity of sulfonamide boronic acids as β-lactamase inhibitors. *Journal of Medicinal Chemistry*, **2010**, 53, 7852-63	8.3	46
93	Identification and optimization of inhibitors of Trypanosomal cysteine proteases: cruzain, rhodesain, and TbCatB. *Journal of Medicinal Chemistry*, **2010**, 53, 52-60	8.3	89
92	Colloid formation by drugs in simulated intestinal fluid. *Journal of Medicinal Chemistry*, **2010**, 53, 4259-65	8.3	62
91	The chemical basis of pharmacology. *Biochemistry*, **2010**, 49, 10267-76	3.2	85
90	The hunt for 8-oxoguanine deaminase. *Journal of the American Chemical Society*, **2010**, 132, 1762-3	16.4	29

89	Rapid context-dependent ligand desolvation in molecular docking. *Journal of Chemical Information and Modeling*, **2010**, 50, 1561-73	6.1	213
88	Quantitative analyses of aggregation, autofluorescence, and reactivity artifacts in a screen for inhibitors of a thiol protease. *Journal of Medicinal Chemistry*, **2010**, 53, 37-51	8.3	164
87	Complementarity between a docking and a high-throughput screen in discovering new cruzain inhibitors. *Journal of Medicinal Chemistry*, **2010**, 53, 4891-905	8.3	155
86	Structure-based discovery of A2A adenosine receptor ligands. *Journal of Medicinal Chemistry*, **2010**, 53, 3748-55	8.3	195
85	Structure-based discovery of beta2-adrenergic receptor ligands. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 6843-8	11.5	265
84	Re-examining the role of Lys67 in class C beta-lactamase catalysis. *Protein Science*, **2009**, 18, 662-9	6.3	22
83	Predicting new molecular targets for known drugs. *Nature*, **2009**, 462, 175-81	50.4	1212
82	Molecular docking and ligand specificity in fragment-based inhibitor discovery. *Nature Chemical Biology*, **2009**, 5, 358-64	11.7	197
81	Quantifying biogenic bias in screening libraries. *Nature Chemical Biology*, **2009**, 5, 479-83	11.7	175
80	Docking and chemoinformatic screens for new ligands and targets. *Current Opinion in Biotechnology* , **2009**, 20, 429-36	11.4	147
79	Functional annotation and three-dimensional structure of Dr0930 from Deinococcus radiodurans, a close relative of phosphotriesterase in the amidohydrolase superfamily. *Biochemistry*, **2009**, 48, 2237-47	3.2	73
78	Predicting ligand binding affinity with alchemical free energy methods in a polar model binding site. *Journal of Molecular Biology*, **2009**, 394, 747-63	6.5	135
77	Divergent modes of enzyme inhibition in a homologous structure-activity series. *Journal of Medicinal Chemistry*, **2009**, 52, 5005-8	8.3	63
76	Molecular docking screens using comparative models of proteins. *Journal of Chemical Information and Modeling*, **2009**, 49, 2512-27	6.1	116
75	Promiscuous aggregate-based inhibitors promote enzyme unfolding. *Journal of Medicinal Chemistry* , **2009**, 52, 2067-75	8.3	163
74	Docking for fragment inhibitors of AmpC beta-lactamase. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 7455-60	11.5	87
73	Automated docking screens: a feasibility study. *Journal of Medicinal Chemistry*, **2009**, 52, 5712-20	8.3	213
72	Small-molecule aggregates inhibit amyloid polymerization. *Nature Chemical Biology*, **2008**, 4, 197-9	11.7	223

71	Stoichiometry and physical chemistry of promiscuous aggregate-based inhibitors. *Journal of the American Chemical Society*, **2008**, 130, 9606-12	16.4	169
70	Rescoring docking hit lists for model cavity sites: predictions and experimental testing. *Journal of Molecular Biology*, **2008**, 377, 914-34	6.5	149
69	Exploiting ordered waters in molecular docking. *Journal of Medicinal Chemistry*, **2008**, 51, 4862-5	8.3	107
68	Quantifying the relationships among drug classes. *Journal of Chemical Information and Modeling*, **2008**, 48, 755-65	6.1	141
67	Comprehensive mechanistic analysis of hits from high-throughput and docking screens against beta-lactamase. *Journal of Medicinal Chemistry*, **2008**, 51, 2502-11	8.3	136
66	Stability and equilibria of promiscuous aggregates in high protein milieus. *Molecular BioSystems*, **2007**, 3, 208-13		58
65	No free energy lunch. *Nature Biotechnology*, **2007**, 25, 1109-10	44.5	9
64	Relating protein pharmacology by ligand chemistry. *Nature Biotechnology*, **2007**, 25, 197-206	44.5	1278
63	Structure-based activity prediction for an enzyme of unknown function. *Nature*, **2007**, 448, 775-9	50.4	216
62	Predicting absolute ligand binding free energies to a simple model site. *Journal of Molecular Biology*, **2007**, 371, 1118-34	6.5	234
61	A high-throughput screen for aggregation-based inhibition in a large compound library. *Journal of Medicinal Chemistry*, **2007**, 50, 2385-90	8.3	288
60	Screening in a spirit haunted world. *Drug Discovery Today*, **2006**, 11, 607-15	8.8	228
59	Interpreting steep dose-response curves in early inhibitor discovery. *Journal of Medicinal Chemistry*, **2006**, 49, 7274-7	8.3	232
58	Prediction of protein-ligand interactions. Docking and scoring: successes and gaps. *Journal of Medicinal Chemistry*, **2006**, 49, 5851-5	8.3	542
57	Benchmarking sets for molecular docking. *Journal of Medicinal Chemistry*, **2006**, 49, 6789-801	8.3	1023
56	The deacylation mechanism of AmpC beta-lactamase at ultrahigh resolution. *Journal of the American Chemical Society*, **2006**, 128, 2970-6	16.4	69
55	Synergy and antagonism of promiscuous inhibition in multiple-compound mixtures. *Journal of Medicinal Chemistry*, **2006**, 49, 2151-4	8.3	65
54	Probing molecular docking in a charged model binding site. *Journal of Molecular Biology*, **2006**, 357, 1449-70	6.5	50

53	A detergent-based assay for the detection of promiscuous inhibitors. *Nature Protocols*, **2006**, 1, 550-3	18.8	335
52	Decoys for docking. *Journal of Medicinal Chemistry*, **2005**, 48, 3714-28	8.3	96
51	Structure, function, and inhibition along the reaction coordinate of CTX-M beta-lactamases. *Journal of the American Chemical Society*, **2005**, 127, 5423-34	16.4	99
50	Atomic resolution structures of CTX-M beta-lactamases: extended spectrum activities from increased mobility and decreased stability. *Journal of Molecular Biology*, **2005**, 348, 349-62	6.5	113
49	ZINC--a free database of commercially available compounds for virtual screening. *Journal of Chemical Information and Modeling*, **2005**, 45, 177-82	6.1	2793
48	Virtual screening against metalloenzymes for inhibitors and substrates. *Biochemistry*, **2005**, 44, 12316-28	3.2	116
47	High-throughput assays for promiscuous inhibitors **2005**, 1, 146-8		261
46	Hierarchical docking of databases of multiple ligand conformations. *Current Topics in Medicinal Chemistry*, **2005**, 5, 739-49	3	120
45	Virtual screening of chemical libraries. *Nature*, **2004**, 432, 862-5	50.4	968
44	Soft docking and multiple receptor conformations in virtual screening. *Journal of Medicinal Chemistry*, **2004**, 47, 5076-84	8.3	199
43	Allosteric inhibition through core disruption. *Journal of Molecular Biology*, **2004**, 336, 1283-91	6.5	107
42	Testing a flexible-receptor docking algorithm in a model binding site. *Journal of Molecular Biology*, **2004**, 337, 1161-82	6.5	164
41	Nanomolar inhibitors of AmpC beta-lactamase. *Journal of the American Chemical Society*, **2003**, 125, 685-95	16.4	111
40	A specific mechanism of nonspecific inhibition. *Journal of Medicinal Chemistry*, **2003**, 46, 4265-72	8.3	529
39	Kinase inhibitors: not just for kinases anymore. *Journal of Medicinal Chemistry*, **2003**, 46, 1478-83	8.3	231
38	Thermodynamic cycle analysis and inhibitor design against beta-lactamase. *Biochemistry*, **2003**, 42, 14483-91	3.2	13
37	Identification and prediction of promiscuous aggregating inhibitors among known drugs. *Journal of Medicinal Chemistry*, **2003**, 46, 4477-86	8.3	428
36	Information decay in molecular docking screens against holo, apo, and modeled conformations of enzymes. *Journal of Medicinal Chemistry*, **2003**, 46, 2895-907	8.3	239

35	Structural milestones in the reaction pathway of an amide hydrolase: substrate, acyl, and product complexes of cephalothin with AmpC beta-lactamase. *Structure*, **2002**, 10, 413-24	5.2	99
34	Structure-based discovery of a novel, noncovalent inhibitor of AmpC beta-lactamase. *Structure*, **2002**, 10, 1013-23	5.2	105
33	Lead discovery using molecular docking. *Current Opinion in Chemical Biology*, **2002**, 6, 439-46	9.7	355
32	Noncovalent interaction energies in covalent complexes: TEM-1 β-lactamase and β-lactams. *Proteins: Structure, Function and Bioinformatics*, **2002**, 47, 86-96	4.2	42
31	Molecular docking and high-throughput screening for novel inhibitors of protein tyrosine phosphatase-1B. *Journal of Medicinal Chemistry*, **2002**, 45, 2213-21	8.3	391
30	Structure-based approach for binding site identification on AmpC beta-lactamase. *Journal of Medicinal Chemistry*, **2002**, 45, 3222-34	8.3	115
29	An ultrahigh resolution structure of TEM-1 beta-lactamase suggests a role for Glu166 as the general base in acylation. *Journal of the American Chemical Society*, **2002**, 124, 5333-40	16.4	173
28	Evolution of an antibiotic resistance enzyme constrained by stability and activity trade-offs. *Journal of Molecular Biology*, **2002**, 320, 85-95	6.5	355
27	Structural bases of stability-function tradeoffs in enzymes. *Journal of Molecular Biology*, **2002**, 321, 285-96	6.5	188
26	A model binding site for testing scoring functions in molecular docking. *Journal of Molecular Biology*, **2002**, 322, 339-55	6.5	178
25	A common mechanism underlying promiscuous inhibitors from virtual and high-throughput screening. *Journal of Medicinal Chemistry*, **2002**, 45, 1712-22	8.3	924
24	Noncovalent interaction energies in covalent complexes: TEM-1 beta-lactamase and beta-lactams. *Proteins: Structure, Function and Bioinformatics*, **2002**, 47, 86-96	4.2	23
23	Docking molecules by families to increase the diversity of hits in database screens: computational strategy and experimental evaluation. *Proteins: Structure, Function and Bioinformatics*, **2001**, 42, 279-93	4.2	47
22	Structures of ceftazidime and its transition-state analogue in complex with AmpC beta-lactamase: implications for resistance mutations and inhibitor design. *Biochemistry*, **2001**, 40, 9207-14	3.2	101
21	Interaction energies between beta-lactam antibiotics and E. coli penicillin-binding protein 5 by reversible thermal denaturation. *Protein Science*, **2001**, 10, 1254-9	6.3	23
20	Inhibition of AmpC beta-lactamase through a destabilizing interaction in the active site. *Biochemistry*, **2001**, 40, 7992-9	3.2	34
19	Crystal Structures of Substrate and Inhibitor Complexes with AmpC β-Lactamase: Possible Implications for Substrate-Assisted Catalysis. *Journal of the American Chemical Society*, **2000**, 122, 10504-10512	16.4	87
18	The complexed structure and antimicrobial activity of a non-beta-lactam inhibitor of AmpC beta-lactamase. *Protein Science*, **1999**, 8, 2330-7	6.3	59

17	Functional analyses of AmpC beta-lactamase through differential stability. *Protein Science*, **1999**, 8, 1816~~24~~	~~6~~	31
16	Ligand solvation in molecular docking. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 4-16	4.2	223
15	Comparing the thermodynamic stabilities of a related thermophilic and mesophilic enzyme. *Biochemistry*, **1999**, 38, 2570-6	3.2	74
14	Ligand solvation in molecular docking **1999**, 34, 4		1
13	Three-dimensional structure of AmpC beta-lactamase from Escherichia coli bound to a transition-state analogue: possible implications for the oxyanion hypothesis and for inhibitor design. *Biochemistry*, **1998**, 37, 16082-92	3.2	101
12	Flexible ligand docking using conformational ensembles. *Protein Science*, **1998**, 7, 938-50	6.3	217
11	Structure-based enhancement of boronic acid-based inhibitors of AmpC beta-lactamase. *Journal of Medicinal Chemistry*, **1998**, 41, 4577-86	8.3	132
10	Enhancement of protein stability by the combination of point mutations in T4 lysozyme is additive. *Protein Engineering, Design and Selection*, **1995**, 8, 1017-22	1.9	85
9	Structure-Based Molecular Design. *Accounts of Chemical Research*, **1994**, 27, 117-123	24.3	297
8	Matching chemistry and shape in molecular docking. *Protein Engineering, Design and Selection*, **1993**, 6, 723-32	1.9	170
7	Molecular docking using shape descriptors. *Journal of Computational Chemistry*, **1992**, 13, 380-397	3.5	348
6	Automated docking with grid-based energy evaluation. *Journal of Computational Chemistry*, **1992**, 13, 505-524	3.5	770
5	Protein docking and complementarity. *Journal of Molecular Biology*, **1991**, 221, 327-46	6.5	264
4	Stereochemical modeling of disulfide bridges. Criteria for introduction into proteins by site-directed mutagenesis. *Protein Engineering, Design and Selection*, **1989**, 3, 95-103	1.9	147
3	Molecular Docking and Structure-Based Design1-23		0
2	Crystal structures of the 2 receptor template large-library docking for selective chemotypes active in vivo		5
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