Brian K Shoichet

List of Publications by Year
in descending order

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193 papers	43,703 citations	2322 98 h-index	2828 191 g-index
210 all docs	210 docs citations	210 times ranked	40007 citing authors

#	Article	IF	Citations
1	Structure-Based Design of a Chemical Probe Set for the 5-HT_{5A} Serotonin Receptor. Journal of Medicinal Chemistry, 2022, 65, 4201-4217.	6.4	17
2	Drug building blocks and libraries at risk in Ukraine. Science, 2022, 376, 929-929.	12.6	1
3	Inactive and active state structures template selective tools for the human 5-HT5A receptor. Nature Structural and Molecular Biology, 2022, 29, 677-687.	8.2	18
4	Property-Unmatched Decoys in Docking Benchmarks. Journal of Chemical Information and Modeling, 2021, 61, 699-714.	5.4	48
5	A Crowding Barrier to Protein Inhibition in Colloidal Aggregates. Journal of Medicinal Chemistry, 2021, 64, 4109-4116.	6.4	7
6	Fragment binding to the Nsp3 macrodomain of SARS-CoV-2 identified through crystallographic screening and computational docking. Science Advances, 2021, 7, .	10.3	100
7	Drug-induced phospholipidosis confounds drug repurposing for SARS-CoV-2. Science, 2021, 373, 541-547.	12.6	148
8	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, .	7.1	17
9	Ligand Strain Energy in Large Library Docking. Journal of Chemical Information and Modeling, 2021, 61, 4331-4341.	5.4	29
10	Efficient Exploration of Chemical Space with Docking and Deep Learning. Journal of Chemical Theory and Computation, 2021, 17, 7106-7119.	5.3	75
11	A practical guide to large-scale docking. Nature Protocols, 2021, 16, 4799-4832.	12.0	206
12	Structure, function and pharmacology of human itch GPCRs. Nature, 2021, 600, 170-175.	27.8	101
13	Colloidal Aggregators in Biochemical SARS-CoV-2 Repurposing Screens. Journal of Medicinal Chemistry, 2021, 64, 17530-17539.	6.4	19
14	Structures of the Ïƒ2 receptor enable docking for bioactive ligand discovery. Nature, 2021, 600, 759-764.	27.8	113
15	Comparative host-coronavirus protein interaction networks reveal pan-viral disease mechanisms. Science, 2020, 370, .	12.6	508
16	The activities of drug inactive ingredients on biological targets. Science, 2020, 369, 403-413.	12.6	61
17	Differential Roles of Extracellular Histidine Residues of GPR68 for Proton-Sensing and Allosteric Modulation by Divalent Metal Ions. Biochemistry, 2020, 59, 3594-3614.	2.5	11
18	Structure of a Hallucinogen-Activated Gq-Coupled 5-HT2A Serotonin Receptor. Cell, 2020, 182, 1574-1588.e19.	28.9	270

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19	An allosteric modulator binds to a conformational hub in the Î²2 adrenergic receptor. Nature Chemical Biology, 2020, 16, 749-755.	8.0	51
20	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.	7.1	39
21	Virtual discovery of melatonin receptor ligands to modulate circadian rhythms. Nature, 2020, 579, 609-614.	27.8	184
22	The Global Phosphorylation Landscape of SARS-CoV-2 Infection. Cell, 2020, 182, 685-712.e19.	28.9	825
23	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. Nature, 2020, 583, 459-468.	27.8	3,542
24	Discovery of Lysine-Targeted eIF4E Inhibitors through Covalent Docking. Journal of the American Chemical Society, 2020, 142, 4960-4964.	13.7	60
25	Interactions of Oral Molecular Excipients with Breast Cancer Resistance Protein, BCRP. Molecular Pharmaceutics, 2020, 17, 748-756.	4.6	16
26	Protein Stability Effects in Aggregate-Based Enzyme Inhibition. Journal of Medicinal Chemistry, 2019, 62, 9593-9599.	6.4	20
27	GAIN domainâ€“mediated cleavage is required for activation of G proteinâ€“coupled receptor 56 (GPR56) by its natural ligands and a small-molecule agonist. Journal of Biological Chemistry, 2019, 294, 19246-19254.	3.4	40
28	Structural identification of a hotspot on CFTR for potentiation. Science, 2019, 364, 1184-1188.	12.6	189
29	Triggered Release Enhances the Cytotoxicity of Stable Colloidal Drug Aggregates. ACS Chemical Biology, 2019, 14, 1507-1514.	3.4	6
30	Colloidal Drug Aggregate Stability in High Serum Conditions and Pharmacokinetic Consequence. ACS Chemical Biology, 2019, 14, 751-757.	3.4	25
31	Ultra-large library docking for discovering new chemotypes. Nature, 2019, 566, 224-229.	27.8	595
32	Structure-based discovery of selective positive allosteric modulators of antagonists for the M ₂ muscarinic acetylcholine receptor. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E2419-E2428.	7.1	57
33	Structure of the D2 dopamine receptor bound to the atypical antipsychotic drug risperidone. Nature, 2018, 555, 269-273.	27.8	341
34	Colloidal aggregation: From screening nuisance to formulation nuance. Nano Today, 2018, 19, 188-200.	11.9	73
35	Structure-inspired design of Î²-arrestin-biased ligands for aminergic GPCRs. Nature Chemical Biology, 2018, 14, 126-134.	8.0	141
36	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.	7.1	64

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37	Far away from the lamppost. PLoS Biology, 2018, 16, e3000067.	5.6	10
38	Prediction of enzymatic pathways by integrative pathway mapping. ELife, 2018, 7, .	6.0	30
39	The Psychiatric Cell Map Initiative: A Convergent Systems Biological Approach to Illuminating Key Molecular Pathways in Neuropsychiatric Disorders. Cell, 2018, 174, 505-520.	28.9	108
40	Selectivity Challenges in Docking Screens for GPCR Targets and Antitargets. Journal of Medicinal Chemistry, 2018, 61, 6830-6845.	6.4	31
41	The Recognition of Unrelated Ligands by Identical Proteins. ACS Chemical Biology, 2018, 13, 2522-2533.	3.4	6
42	Crystal Structure of an LSD-Bound Human Serotonin Receptor. Cell, 2017, 168, 377-389.e12.	28.9	340
43	Leveraging Colloidal Aggregation for Drug-Rich Nanoparticle Formulations. Molecular Pharmaceutics, 2017, 14, 1852-1860.	4.6	16
44	In silico design of novel probes for the atypical opioid receptor MRGPRX2. Nature Chemical Biology, 2017, 13, 529-536.	8.0	230
45	A New Spin on Antibodyâ€“Drug Conjugates: Trastuzumab-Fulvestrant Colloidal Drug Aggregates Target HER2-Positive Cells. ACS Applied Materials & Interfaces, 2017, 9, 12195-12202.	8.0	24
46	Internal Structure and Preferential Protein Binding of Colloidal Aggregates. ACS Chemical Biology, 2017, 12, 282-290.	3.4	26
47	Structure-Based Design and Discovery of New M₂ Receptor Agonists. Journal of Medicinal Chemistry, 2017, 60, 9239-9250.	6.4	19
48	Discovery of new GPCR ligands to illuminate new biology. Nature Chemical Biology, 2017, 13, 1143-1151.	8.0	80
49	D ₄ dopamine receptor high-resolution structures enable the discovery of selective agonists. Science, 2017, 358, 381-386.	12.6	176
50	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.	7.1	65
51	Reverse translation of adverse event reports paves the way for de-risking preclinical off-targets. ELife, 2017, 6, .	6.0	44
52	In Vitro and In Vivo Characterization of the Alkaloid Nuciferine. PLoS ONE, 2016, 11, e0150602.	2.5	28
53	Identification of Novel Smoothened Ligands Using Structure-Based Docking. PLoS ONE, 2016, 11, e0160365.	2.5	17
54	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, 12021-12024.	13.7	61

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55	Design, Synthesis, and Biological Evaluation of Novel Tetrahydroprotoberberine Derivatives (THPBs) as Selective Î±_{1A}-Adrenoceptor Antagonists. Journal of Medicinal Chemistry, 2016, 59, 9489-9502.	6.4	23
56	Structure-based discovery of opioid analgesics with reduced side effects. Nature, 2016, 537, 185-190.	27.8	744
57	Docking Screens for Novel Ligands Conferring New Biology. Journal of Medicinal Chemistry, 2016, 59, 4103-4120.	6.4	218
58	Stable Colloidal Drug Aggregates Catch and Release Active Enzymes. ACS Chemical Biology, 2016, 11, 992-1000.	3.4	36
59	Docking and Linking of Fragments To Discover Jumonji Histone Demethylase Inhibitors. Journal of Medicinal Chemistry, 2016, 59, 1580-1598.	6.4	43
60	Ligand Similarity Complements Sequence, Physical Interaction, and Co-Expression for Gene Function Prediction. PLoS ONE, 2016, 11, e0160098.	2.5	10
61	One Crystal, Two Temperatures: Cryocooling Penalties Alter Ligand Binding to Transient Protein Sites. ChemBioChem, 2015, 16, 1560-1564.	2.6	76
62	Colloidal Aggregation and the in Vitro Activity of Traditional Chinese Medicines. ACS Chemical Biology, 2015, 10, 978-988.	3.4	58
63	Virtual Screening for UDP-Galactopyranose Mutase Ligands Identifies a New Class of Antimycobacterial Agents. ACS Chemical Biology, 2015, 10, 2209-2218.	3.4	34
64	The promise and peril of chemical probes. Nature Chemical Biology, 2015, 11, 536-541.	8.0	698
65	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, 5039-5044.	7.1	43
66	The Recognition of Identical Ligands by Unrelated Proteins. ACS Chemical Biology, 2015, 10, 2772-2784.	3.4	70
67	Activity-Independent Discovery of Secondary Metabolites Using Chemical Elicitation and Cheminformatic Inference. ACS Chemical Biology, 2015, 10, 2616-2623.	3.4	43
68	Small-Molecule Allosteric Modulators of the Protein Kinase PDK1 from Structure-Based Docking. Journal of Medicinal Chemistry, 2015, 58, 8285-8291.	6.4	32
69	An Aggregation Advisor for Ligand Discovery. Journal of Medicinal Chemistry, 2015, 58, 7076-7087.	6.4	350
70	Prediction and validation of enzyme and transporter off-targets for metformin. Journal of Pharmacokinetics and Pharmacodynamics, 2015, 42, 463-475.	1.8	37
71	Allosteric ligands for the pharmacologically dark receptors GPR68 and GPR65. Nature, 2015, 527, 477-483.	27.8	214
72	Follow your lead. Nature Chemical Biology, 2014, 10, 244-245.	8.0	10

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73	Large-Scale Identification and Analysis of Suppressive Drug Interactions. Chemistry and Biology, 2014, 21, 541-551.	6.0	27
74	Incorporation of protein flexibility and conformational energy penalties in docking screens to improve ligand discovery. Nature Chemistry, 2014, 6, 575-583.	13.6	124
75	Covalent docking of large libraries for the discovery of chemical probes. Nature Chemical Biology, 2014, 10, 1066-1072.	8.0	225
76	Colloidal Drug Formulations Can Explain â€œBell-Shapedâ€•Concentrationâ€“Response Curves. ACS Chemical Biology, 2014, 9, 777-784.	3.4	106
77	Actin Is Required for IFT Regulation in Chlamydomonas reinhardtii. Current Biology, 2014, 24, 2025-2032.	3.9	66
78	Functional Annotation and Structural Characterization of a Novel Lactonase Hydrolyzing <scp>d</scp>-Xylono-1,4-lactone-5-phosphate and <scp>l</scp>-Arabino-1,4-lactone-5-phosphate. Biochemistry, 2014, 53, 4727-4738.	2.5	10
79	Increasing Chemical Space Coverage by Combining Empirical and Computational Fragment Screens. ACS Chemical Biology, 2014, 9, 1528-1535.	3.4	58
80	Blind Prediction of Charged Ligand Binding Affinities in a Model Binding Site. Journal of Molecular Biology, 2013, 425, 4569-4583.	4.2	53
81	Chemical informatics uncovers a new role for moexipril as a novel inhibitor of cAMP phosphodiesterase-4 (PDE4). Biochemical Pharmacology, 2013, 85, 1297-1305.	4.4	17
82	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.	13.7	32
83	A pharmacological organization of G proteinâ€“coupled receptors. Nature Methods, 2013, 10, 140-146.	19.0	89
84	Colloidal Aggregation Causes Inhibition of G Protein-Coupled Receptors. Journal of Medicinal Chemistry, 2013, 56, 2406-2414.	6.4	91
85	The Impact of Introducing a Histidine into an Apolar Cavity Site on Docking and Ligand Recognition. Journal of Medicinal Chemistry, 2013, 56, 2874-2884.	6.4	10
86	Functional Annotation and Three-Dimensional Structure of an Incorrectly Annotated Dihydroorotase from cog3964 in the Amidohydrolase Superfamily. Biochemistry, 2013, 52, 228-238.	2.5	8
87	Muscarinic Receptors as Model Targets and Antitargets for Structure-Based Ligand Discovery. Molecular Pharmacology, 2013, 84, 528-540.	2.3	56
88	Roles for Ordered and Bulk Solvent in Ligand Recognition and Docking in Two Related Cavities. PLoS ONE, 2013, 8, e69153.	2.5	23
89	Ligand Pose and Orientational Sampling in Molecular Docking. PLoS ONE, 2013, 8, e75992.	2.5	139
90	Structure-based ligand discovery for the proteinâ€“protein interface of chemokine receptor CXCR4. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 5517-5522.	7.1	140

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91	Identifying mechanism-of-action targets for drugs and probes. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 11178-11183.	7.1	156
92	Fragment-guided design of subnanomolar Î²-lactamase inhibitors active in vivo. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 17448-17453.	7.1	67
93	Structure-based drug screening for G-protein-coupled receptors. Trends in Pharmacological Sciences, 2012, 33, 268-272.	8.7	258
94	Directory of Useful Decoys, Enhanced (DUD-E): Better Ligands and Decoys for Better Benchmarking. Journal of Medicinal Chemistry, 2012, 55, 6582-6594.	6.4	1,574
95	Large-scale prediction and testing of drug activity on side-effect targets. Nature, 2012, 486, 361-367.	27.8	782
96	Colloidal Aggregation Affects the Efficacy of Anticancer Drugs in Cell Culture. ACS Chemical Biology, 2012, 7, 1429-1435.	3.4	148
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, 15810-15815.	7.1	120
98	The Enzyme Function Initiative. Biochemistry, 2011, 50, 9950-9962.	2.5	169
99	Ligand discovery from a dopamine D3 receptor homology model and crystal structure. Nature Chemical Biology, 2011, 7, 769-778.	8.0	285
100	Statistical Potential for Modeling and Ranking of Proteinâ€“Ligand Interactions. Journal of Chemical Information and Modeling, 2011, 51, 3078-3092.	5.4	69
101	Rapid behavior-based identification of neuroactive small molecules in the zebrafish. Nature Chemical Biology, 2010, 6, 231-237.	8.0	482
102	Design, Synthesis, Crystal Structures, and Antimicrobial Activity of Sulfonamide Boronic Acids as Î²-Lactamase Inhibitors. Journal of Medicinal Chemistry, 2010, 53, 7852-7863.	6.4	53
103	Identification and Optimization of Inhibitors of Trypanosomal Cysteine Proteases: Cruzain, Rhodesain, and TbCatB. Journal of Medicinal Chemistry, 2010, 53, 52-60.	6.4	103
104	Colloid Formation by Drugs in Simulated Intestinal Fluid. Journal of Medicinal Chemistry, 2010, 53, 4259-4265.	6.4	72
105	The Chemical Basis of Pharmacology. Biochemistry, 2010, 49, 10267-10276.	2.5	93
106	The Hunt for 8-Oxoguanine Deaminase. Journal of the American Chemical Society, 2010, 132, 1762-1763.	13.7	34
107	Rapid Context-Dependent Ligand Desolvation in Molecular Docking. Journal of Chemical Information and Modeling, 2010, 50, 1561-1573.	5.4	276
108	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.	6.4	213

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109	Complementarity Between a Docking and a High-Throughput Screen in Discovering New Cruzain Inhibitors. Journal of Medicinal Chemistry, 2010, 53, 4891-4905.	6.4	199
110	Structure-Based Discovery of A_{2A}Adenosine Receptor Ligands. Journal of Medicinal Chemistry, 2010, 53, 3748-3755.	6.4	212
111	Structure-based discovery of Î² ₂ -adrenergic receptor ligands. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 6843-6848.	7.1	290
112	Reâ€examining the role of Lys67 in class C Î²â€lactamase catalysis. Protein Science, 2009, 18, 662-669.	7.6	32
113	Predicting new molecular targets for known drugs. Nature, 2009, 462, 175-181.	27.8	1,474
114	Molecular docking and ligand specificity in fragment-based inhibitor discovery. Nature Chemical Biology, 2009, 5, 358-364.	8.0	225
115	Quantifying biogenic bias in screening libraries. Nature Chemical Biology, 2009, 5, 479-483.	8.0	198
116	Docking and chemoinformatic screens for new ligands and targets. Current Opinion in Biotechnology, 2009, 20, 429-436.	6.6	168
117	Functional Annotation and Three-Dimensional Structure of Dr0930 from Deinococcus radiodurans, a Close Relative of Phosphotriesterase in the Amidohydrolase Superfamily. Biochemistry, 2009, 48, 2237-2247.	2.5	82
118	Predicting Ligand Binding Affinity with Alchemical Free Energy Methods in a Polar Model Binding Site. Journal of Molecular Biology, 2009, 394, 747-763.	4.2	160
119	Divergent Modes of Enzyme Inhibition in a Homologous Structureâ^'Activity Series. Journal of Medicinal Chemistry, 2009, 52, 5005-5008.	6.4	84
120	Molecular Docking Screens Using Comparative Models of Proteins. Journal of Chemical Information and Modeling, 2009, 49, 2512-2527.	5.4	132
121	Promiscuous Aggregate-Based Inhibitors Promote Enzyme Unfolding. Journal of Medicinal Chemistry, 2009, 52, 2067-2075.	6.4	183
122	Docking for fragment inhibitors of AmpC Î²-lactamase. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 7455-7460.	7.1	101
123	Automated Docking Screens: A Feasibility Study. Journal of Medicinal Chemistry, 2009, 52, 5712-5720.	6.4	245
124	Small-molecule aggregates inhibit amyloid polymerization. Nature Chemical Biology, 2008, 4, 197-199.	8.0	244
125	Stoichiometry and Physical Chemistry of Promiscuous Aggregate-Based Inhibitors. Journal of the American Chemical Society, 2008, 130, 9606-9612.	13.7	200
126	Rescoring Docking Hit Lists for Model Cavity Sites: Predictions and Experimental Testing. Journal of Molecular Biology, 2008, 377, 914-934.	4.2	168

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127	Exploiting Ordered Waters in Molecular Docking. Journal of Medicinal Chemistry, 2008, 51, 4862-4865.	6.4	117
128	Quantifying the Relationships among Drug Classes. Journal of Chemical Information and Modeling, 2008, 48, 755-765.	5.4	160
129	Comprehensive Mechanistic Analysis of Hits from High-Throughput and Docking Screens against Î²-Lactamase. Journal of Medicinal Chemistry, 2008, 51, 2502-2511.	6.4	169
130	Predicting Absolute Ligand Binding Free Energies to a Simple Model Site. Journal of Molecular Biology, 2007, 371, 1118-1134.	4.2	269
131	A High-Throughput Screen for Aggregation-Based Inhibition in a Large Compound Library. Journal of Medicinal Chemistry, 2007, 50, 2385-2390.	6.4	332
132	Stability and equilibria of promiscuous aggregates in high protein milieus. Molecular BioSystems, 2007, 3, 208.	2.9	67
133	No free energy lunch. Nature Biotechnology, 2007, 25, 1109-1110.	17.5	14
134	Relating protein pharmacology by ligand chemistry. Nature Biotechnology, 2007, 25, 197-206.	17.5	1,722
135	Structure-based activity prediction for an enzyme of unknown function. Nature, 2007, 448, 775-779.	27.8	249
136	Interpreting Steep Dose-Response Curves in Early Inhibitor Discovery. Journal of Medicinal Chemistry, 2006, 49, 7274-7277.	6.4	268
137	Prediction of Proteinâ^'Ligand Interactions. Docking and Scoring:Â Successes and Gaps. Journal of Medicinal Chemistry, 2006, 49, 5851-5855.	6.4	603
138	Benchmarking Sets for Molecular Docking. Journal of Medicinal Chemistry, 2006, 49, 6789-6801.	6.4	1,184
139	The Deacylation Mechanism of AmpC Î²-Lactamase at Ultrahigh Resolution. Journal of the American Chemical Society, 2006, 128, 2970-2976.	13.7	78
140	Synergy and Antagonism of Promiscuous Inhibition in Multiple-Compound Mixtures. Journal of Medicinal Chemistry, 2006, 49, 2151-2154.	6.4	72
141	Probing Molecular Docking in a Charged Model Binding Site. Journal of Molecular Biology, 2006, 357, 1449-1470.	4.2	61
142	A detergent-based assay for the detection of promiscuous inhibitors. Nature Protocols, 2006, 1, 550-553.	12.0	397
143	Screening in a spirit haunted world. Drug Discovery Today, 2006, 11, 607-615.	6.4	265
144	High-throughput assays for promiscuous inhibitors. , 2005, 1, 146-148.		300

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145	Hierarchical Docking of Databases of Multiple Ligand Conformations. Current Topics in Medicinal Chemistry, 2005, 5, 739-749.	2.1	139
146	Decoys for Docking. Journal of Medicinal Chemistry, 2005, 48, 3714-3728.	6.4	107
147	Structure, Function, and Inhibition along the Reaction Coordinate of CTX-M Î²-Lactamases. Journal of the American Chemical Society, 2005, 127, 5423-5434.	13.7	114
148	Atomic Resolution Structures of CTX-M Î²-Lactamases: Extended Spectrum Activities from Increased Mobility and Decreased Stability. Journal of Molecular Biology, 2005, 348, 349-362.	4.2	134
149	ZINC â^' A Free Database of Commercially Available Compounds for Virtual Screening. Journal of Chemical Information and Modeling, 2005, 45, 177-182.	5.4	3,366
150	Virtual Screening against Metalloenzymes for Inhibitors and Substratesâ€. Biochemistry, 2005, 44, 12316-12328.	2.5	125
151	Virtual screening of chemical libraries. Nature, 2004, 432, 862-865.	27.8	1,175
152	Soft Docking and Multiple Receptor Conformations in Virtual Screening. Journal of Medicinal Chemistry, 2004, 47, 5076-5084.	6.4	228
153	Allosteric Inhibition Through Core Disruption. Journal of Molecular Biology, 2004, 336, 1283-1291.	4.2	132
154	Testing a Flexible-receptor Docking Algorithm in a Model Binding Site. Journal of Molecular Biology, 2004, 337, 1161-1182.	4.2	184
155	Nanomolar Inhibitors of AmpC Î²-Lactamase. Journal of the American Chemical Society, 2003, 125, 685-695.	13.7	123
156	A Specific Mechanism of Nonspecific Inhibition. Journal of Medicinal Chemistry, 2003, 46, 4265-4272.	6.4	583
157	Kinase Inhibitors:â€‰ Not Just for Kinases Anymore. Journal of Medicinal Chemistry, 2003, 46, 1478-1483.	6.4	245
158	Thermodynamic Cycle Analysis and Inhibitor Design against Beta-Lactamaseâ€. Biochemistry, 2003, 42, 14483-14491.	2.5	14
159	Identification and Prediction of Promiscuous Aggregating Inhibitors among Known Drugs. Journal of Medicinal Chemistry, 2003, 46, 4477-4486.	6.4	467
160	Information Decay in Molecular Docking Screens against Holo, Apo, and Modeled Conformations of Enzymes. Journal of Medicinal Chemistry, 2003, 46, 2895-2907.	6.4	266
161	Structure-Based Approach for Binding Site Identification on AmpC Î²-Lactamase. Journal of Medicinal Chemistry, 2002, 45, 3222-3234.	6.4	123
162	An Ultrahigh Resolution Structure of TEM-1 Î²-Lactamase Suggests a Role for Glu166 as the General Base in Acylation. Journal of the American Chemical Society, 2002, 124, 5333-5340.	13.7	205

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163	Evolution of an Antibiotic Resistance Enzyme Constrained by Stability and Activity Trade-offs. Journal of Molecular Biology, 2002, 320, 85-95.	4.2	421
164	Structural Bases of Stabilityâ€“function Tradeoffs in Enzymes. Journal of Molecular Biology, 2002, 321, 285-296.	4.2	221
165	A Model Binding Site for Testing Scoring Functions in Molecular Docking. Journal of Molecular Biology, 2002, 322, 339-355.	4.2	212
166	A Common Mechanism Underlying Promiscuous Inhibitors from Virtual and High-Throughput Screening. Journal of Medicinal Chemistry, 2002, 45, 1712-1722.	6.4	1,013
167	Structural Milestones in the Reaction Pathway of an Amide Hydrolase. Structure, 2002, 10, 413-424.	3.3	104
168	Structure-Based Discovery of a Novel, Noncovalent Inhibitor of AmpC Î²-Lactamase. Structure, 2002, 10, 1013-1023.	3.3	119
169	Lead discovery using molecular docking. Current Opinion in Chemical Biology, 2002, 6, 439-446.	6.1	429
170	Noncovalent interaction energies in covalent complexes: TEM-1 ?-lactamase and ?-lactams. Proteins: Structure, Function and Bioinformatics, 2002, 47, 86-96.	2.6	48
171	Molecular Docking and High-Throughput Screening for Novel Inhibitors of Protein Tyrosine Phosphatase-1B. Journal of Medicinal Chemistry, 2002, 45, 2213-2221.	6.4	453
172	Noncovalent interaction energies in covalent complexes: TEM-1 beta-lactamase and beta-lactams. Proteins: Structure, Function and Bioinformatics, 2002, 47, 86-96.	2.6	24
173	Inhibition of AmpC Î²-Lactamase through a Destabilizing Interaction in the Active Site,. Biochemistry, 2001, 40, 7992-7999.	2.5	36
174	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, 279-293.	2.6	51
175	Structures of Ceftazidime and Its Transition-State Analogue in Complex with AmpC Î²-Lactamase:â€‰ Implications for Resistance Mutations and Inhibitor Design,. Biochemistry, 2001, 40, 9207-9214.	2.5	112
176	Interaction energies between Î²-lactam antibiotics and E. coli penicillin-binding protein 5 by reversible thermal denaturation. Protein Science, 2001, 10, 1254-1259.	7.6	23
177	Crystal Structures of Substrate and Inhibitor Complexes with AmpC Î²-Lactamase:Â Possible Implications for Substrate-Assisted Catalysis. Journal of the American Chemical Society, 2000, 122, 10504-10512.	13.7	92
178	Functional analyses of AmpC Î²â€lactamase through differential stability. Protein Science, 1999, 8, 1816-1824.	7.6	34
179	Ligand solvation in molecular docking. Proteins: Structure, Function and Bioinformatics, 1999, 34, 4-16.	2.6	252
180	Comparing the Thermodynamic Stabilities of a Related Thermophilic and Mesophilic Enzymeâ€. Biochemistry, 1999, 38, 2570-2576.	2.5	78

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181	The complexed structure and antimicrobial activity of a nonâ€Î²â€lactam inhibitor of AmpC Î²â€lactamase. Protein Science, 1999, 8, 2330-2337.	7.6	66
182	Ligand solvation in molecular docking. , 1999, 34, 4.		1
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