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	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. Nature, 2020, 583, 459-468.	27.8	3,542
2	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
3	Relating protein pharmacology by ligand chemistry. Nature Biotechnology, 2007, 25, 197-206.	17.5	1,722
4	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
5	Predicting new molecular targets for known drugs. Nature, 2009, 462, 175-181.	27.8	1,474
6	Benchmarking Sets for Molecular Docking. Journal of Medicinal Chemistry, 2006, 49, 6789-6801.	6.4	1,184
7	Virtual screening of chemical libraries. Nature, 2004, 432, 862-865.	27.8	1,175
8	A Common Mechanism Underlying Promiscuous Inhibitors from Virtual and High-Throughput Screening. Journal of Medicinal Chemistry, 2002, 45, 1712-1722.	6.4	1,013
9	Automated docking with grid-based energy evaluation. Journal of Computational Chemistry, 1992, 13, 505-524.	3.3	900
10	The Global Phosphorylation Landscape of SARS-CoV-2 Infection. Cell, 2020, 182, 685-712.e19.	28.9	825
11	Large-scale prediction and testing of drug activity on side-effect targets. Nature, 2012, 486, 361-367.	27.8	782
12	Structure-based discovery of opioid analgesics with reduced side effects. Nature, 2016, 537, 185-190.	27.8	744
13	The promise and peril of chemical probes. Nature Chemical Biology, 2015, 11, 536-541.	8.0	698
14	Prediction of Proteinâ^'Ligand Interactions. Docking and Scoring:Â Successes and Gaps. Journal of Medicinal Chemistry, 2006, 49, 5851-5855.	6.4	603
15	Ultra-large library docking for discovering new chemotypes. Nature, 2019, 566, 224-229.	27.8	595
16	A Specific Mechanism of Nonspecific Inhibition. Journal of Medicinal Chemistry, 2003, 46, 4265-4272.	6.4	583
17	Comparative host-coronavirus protein interaction networks reveal pan-viral disease mechanisms. Science, 2020, 370, .	12.6	508
18	Rapid behavior-based identification of neuroactive small molecules in the zebrafish. Nature Chemical Biology, 2010, 6, 231-237.	8.0	482

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19	Identification and Prediction of Promiscuous Aggregating Inhibitors among Known Drugs. Journal of Medicinal Chemistry, 2003, 46, 4477-4486.	6.4	467
20	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
21	Lead discovery using molecular docking. Current Opinion in Chemical Biology, 2002, 6, 439-446.	6.1	429
22	Evolution of an Antibiotic Resistance Enzyme Constrained by Stability and Activity Trade-offs. Journal of Molecular Biology, 2002, 320, 85-95.	4.2	421
23	A detergent-based assay for the detection of promiscuous inhibitors. Nature Protocols, 2006, 1, 550-553.	12.0	397
24	Molecular docking using shape descriptors. Journal of Computational Chemistry, 1992, 13, 380-397.	3.3	393
25	An Aggregation Advisor for Ligand Discovery. Journal of Medicinal Chemistry, 2015, 58, 7076-7087.	6.4	350
26	Structure of the D2 dopamine receptor bound to the atypical antipsychotic drug risperidone. Nature, 2018, 555, 269-273.	27.8	341
27	Crystal Structure of an LSD-Bound Human Serotonin Receptor. Cell, 2017, 168, 377-389.e12.	28.9	340
28	Structure-Based Molecular Design. Accounts of Chemical Research, 1994, 27, 117-123.	15.6	339
29	A High-Throughput Screen for Aggregation-Based Inhibition in a Large Compound Library. Journal of Medicinal Chemistry, 2007, 50, 2385-2390.	6.4	332
30	High-throughput assays for promiscuous inhibitors. , 2005, 1, 146-148.		300
31	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
32	Protein docking and complementarity. Journal of Molecular Biology, 1991, 221, 327-346.	4.2	287
33	Ligand discovery from a dopamine D3 receptor homology model and crystal structure. Nature Chemical Biology, 2011, 7, 769-778.	8.0	285
34	Rapid Context-Dependent Ligand Desolvation in Molecular Docking. Journal of Chemical Information and Modeling, 2010, 50, 1561-1573.	5.4	276
35	Structure of a Hallucinogen-Activated Gq-Coupled 5-HT2A Serotonin Receptor. Cell, 2020, 182, 1574-1588.e19.	28.9	270
36	Predicting Absolute Ligand Binding Free Energies to a Simple Model Site. Journal of Molecular Biology, 2007, 371, 1118-1134.	4.2	269

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37	Interpreting Steep Dose-Response Curves in Early Inhibitor Discovery. Journal of Medicinal Chemistry, 2006, 49, 7274-7277.	6.4	268
38	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
39	Screening in a spirit haunted world. Drug Discovery Today, 2006, 11, 607-615.	6.4	265
40	Structure-based drug screening for G-protein-coupled receptors. Trends in Pharmacological Sciences, 2012, 33, 268-272.	8.7	258
41	Flexible ligand docking using conformational ensembles. Protein Science, 1998, 7, 938-950.	7.6	252
42	Ligand solvation in molecular docking. Proteins: Structure, Function and Bioinformatics, 1999, 34, 4-16.	2.6	252
43	Structure-based activity prediction for an enzyme of unknown function. Nature, 2007, 448, 775-779.	27.8	249
44	Kinase Inhibitors:â€‰ Not Just for Kinases Anymore. Journal of Medicinal Chemistry, 2003, 46, 1478-1483.	6.4	245
45	Automated Docking Screens: A Feasibility Study. Journal of Medicinal Chemistry, 2009, 52, 5712-5720.	6.4	245
46	Small-molecule aggregates inhibit amyloid polymerization. Nature Chemical Biology, 2008, 4, 197-199.	8.0	244
47	In silico design of novel probes for the atypical opioid receptor MRGPRX2. Nature Chemical Biology, 2017, 13, 529-536.	8.0	230
48	Soft Docking and Multiple Receptor Conformations in Virtual Screening. Journal of Medicinal Chemistry, 2004, 47, 5076-5084.	6.4	228
49	Molecular docking and ligand specificity in fragment-based inhibitor discovery. Nature Chemical Biology, 2009, 5, 358-364.	8.0	225
50	Covalent docking of large libraries for the discovery of chemical probes. Nature Chemical Biology, 2014, 10, 1066-1072.	8.0	225
51	Structural Bases of Stabilityâ€“function Tradeoffs in Enzymes. Journal of Molecular Biology, 2002, 321, 285-296.	4.2	221
52	Docking Screens for Novel Ligands Conferring New Biology. Journal of Medicinal Chemistry, 2016, 59, 4103-4120.	6.4	218
53	Allosteric ligands for the pharmacologically dark receptors GPR68 and GPR65. Nature, 2015, 527, 477-483.	27.8	214
54	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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55	A Model Binding Site for Testing Scoring Functions in Molecular Docking. Journal of Molecular Biology, 2002, 322, 339-355.	4.2	212
56	Structure-Based Discovery of A_{2A}Adenosine Receptor Ligands. Journal of Medicinal Chemistry, 2010, 53, 3748-3755.	6.4	212
57	A practical guide to large-scale docking. Nature Protocols, 2021, 16, 4799-4832.	12.0	206
58	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
59	Stoichiometry and Physical Chemistry of Promiscuous Aggregate-Based Inhibitors. Journal of the American Chemical Society, 2008, 130, 9606-9612.	13.7	200
60	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
61	Quantifying biogenic bias in screening libraries. Nature Chemical Biology, 2009, 5, 479-483.	8.0	198
62	Structural identification of a hotspot on CFTR for potentiation. Science, 2019, 364, 1184-1188.	12.6	189
63	Testing a Flexible-receptor Docking Algorithm in a Model Binding Site. Journal of Molecular Biology, 2004, 337, 1161-1182.	4.2	184
64	Virtual discovery of melatonin receptor ligands to modulate circadian rhythms. Nature, 2020, 579, 609-614.	27.8	184
65	Promiscuous Aggregate-Based Inhibitors Promote Enzyme Unfolding. Journal of Medicinal Chemistry, 2009, 52, 2067-2075.	6.4	183
66	Matching chemistry and shape in molecular docking. Protein Engineering, Design and Selection, 1993, 6, 723-732.	2.1	182
67	D ₄ dopamine receptor high-resolution structures enable the discovery of selective agonists. Science, 2017, 358, 381-386.	12.6	176
68	Stereochemical modeling of disulfide bridges. Criteria for introduction into proteins by site-directed mutagenesis. Protein Engineering, Design and Selection, 1989, 3, 95-103.	2.1	171
69	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
70	The Enzyme Function Initiative. Biochemistry, 2011, 50, 9950-9962.	2.5	169
71	Rescoring Docking Hit Lists for Model Cavity Sites: Predictions and Experimental Testing. Journal of Molecular Biology, 2008, 377, 914-934.	4.2	168
72	Docking and chemoinformatic screens for new ligands and targets. Current Opinion in Biotechnology, 2009, 20, 429-436.	6.6	168

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73	Quantifying the Relationships among Drug Classes. Journal of Chemical Information and Modeling, 2008, 48, 755-765.	5.4	160
74	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
75	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
76	Colloidal Aggregation Affects the Efficacy of Anticancer Drugs in Cell Culture. ACS Chemical Biology, 2012, 7, 1429-1435.	3.4	148
77	Drug-induced phospholipidosis confounds drug repurposing for SARS-CoV-2. Science, 2021, 373, 541-547.	12.6	148
78	Structure-inspired design of Î²-arrestin-biased ligands for aminergic GPCRs. Nature Chemical Biology, 2018, 14, 126-134.	8.0	141
79	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
80	Structure-Based Enhancement of Boronic Acid-Based Inhibitors of AmpC Î²-Lactamase. Journal of Medicinal Chemistry, 1998, 41, 4577-4586.	6.4	139
81	Hierarchical Docking of Databases of Multiple Ligand Conformations. Current Topics in Medicinal Chemistry, 2005, 5, 739-749.	2.1	139
82	Ligand Pose and Orientational Sampling in Molecular Docking. PLoS ONE, 2013, 8, e75992.	2.5	139
83	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
84	Allosteric Inhibition Through Core Disruption. Journal of Molecular Biology, 2004, 336, 1283-1291.	4.2	132
85	Molecular Docking Screens Using Comparative Models of Proteins. Journal of Chemical Information and Modeling, 2009, 49, 2512-2527.	5.4	132
86	Virtual Screening against Metalloenzymes for Inhibitors and Substratesâ€. Biochemistry, 2005, 44, 12316-12328.	2.5	125
87	Incorporation of protein flexibility and conformational energy penalties in docking screens to improve ligand discovery. Nature Chemistry, 2014, 6, 575-583.	13.6	124
88	Structure-Based Approach for Binding Site Identification on AmpC Î²-Lactamase. Journal of Medicinal Chemistry, 2002, 45, 3222-3234.	6.4	123
89	Nanomolar Inhibitors of AmpC Î²-Lactamase. Journal of the American Chemical Society, 2003, 125, 685-695.	13.7	123
90	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

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91	Structure-Based Discovery of a Novel, Noncovalent Inhibitor of AmpC Î²-Lactamase. Structure, 2002, 10, 1013-1023.	3.3	119
92	Exploiting Ordered Waters in Molecular Docking. Journal of Medicinal Chemistry, 2008, 51, 4862-4865.	6.4	117
93	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
94	Three-Dimensional Structure of AmpC Î²-Lactamase fromEscherichiacoliBound to a Transition-State Analogue:Â Possible Implications for the Oxyanion Hypothesis and for Inhibitor Designâ€. Biochemistry, 1998, 37, 16082-16092.	2.5	113
95	Structures of the Ïƒ2 receptor enable docking for bioactive ligand discovery. Nature, 2021, 600, 759-764.	27.8	113
96	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
97	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
98	Decoys for Docking. Journal of Medicinal Chemistry, 2005, 48, 3714-3728.	6.4	107
99	Colloidal Drug Formulations Can Explain â€œBell-Shapedâ€•Concentrationâ€“Response Curves. ACS Chemical Biology, 2014, 9, 777-784.	3.4	106
100	Structural Milestones in the Reaction Pathway of an Amide Hydrolase. Structure, 2002, 10, 413-424.	3.3	104
101	Enhancement of protein stability by the combination of point mutations in T4 lysozyme is additive. Protein Engineering, Design and Selection, 1995, 8, 1017-1022.	2.1	103
102	Identification and Optimization of Inhibitors of Trypanosomal Cysteine Proteases: Cruzain, Rhodesain, and TbCatB. Journal of Medicinal Chemistry, 2010, 53, 52-60.	6.4	103
103	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
104	Structure, function and pharmacology of human itch GPCRs. Nature, 2021, 600, 170-175.	27.8	101
105	Fragment binding to the Nsp3 macrodomain of SARS-CoV-2 identified through crystallographic screening and computational docking. Science Advances, 2021, 7, .	10.3	100
106	The Chemical Basis of Pharmacology. Biochemistry, 2010, 49, 10267-10276.	2.5	93
107	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
108	Colloidal Aggregation Causes Inhibition of G Protein-Coupled Receptors. Journal of Medicinal Chemistry, 2013, 56, 2406-2414.	6.4	91

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109	A pharmacological organization of G proteinâ€“coupled receptors. Nature Methods, 2013, 10, 140-146.	19.0	89
110	Divergent Modes of Enzyme Inhibition in a Homologous Structureâ^'Activity Series. Journal of Medicinal Chemistry, 2009, 52, 5005-5008.	6.4	84
111	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
112	Discovery of new GPCR ligands to illuminate new biology. Nature Chemical Biology, 2017, 13, 1143-1151.	8.0	80
113	Comparing the Thermodynamic Stabilities of a Related Thermophilic and Mesophilic Enzymeâ€. Biochemistry, 1999, 38, 2570-2576.	2.5	78
114	The Deacylation Mechanism of AmpC Î²-Lactamase at Ultrahigh Resolution. Journal of the American Chemical Society, 2006, 128, 2970-2976.	13.7	78
115	One Crystal, Two Temperatures: Cryocooling Penalties Alter Ligand Binding to Transient Protein Sites. ChemBioChem, 2015, 16, 1560-1564.	2.6	76
116	Efficient Exploration of Chemical Space with Docking and Deep Learning. Journal of Chemical Theory and Computation, 2021, 17, 7106-7119.	5.3	75
117	Colloidal aggregation: From screening nuisance to formulation nuance. Nano Today, 2018, 19, 188-200.	11.9	73
118	Synergy and Antagonism of Promiscuous Inhibition in Multiple-Compound Mixtures. Journal of Medicinal Chemistry, 2006, 49, 2151-2154.	6.4	72
119	Colloid Formation by Drugs in Simulated Intestinal Fluid. Journal of Medicinal Chemistry, 2010, 53, 4259-4265.	6.4	72
120	The Recognition of Identical Ligands by Unrelated Proteins. ACS Chemical Biology, 2015, 10, 2772-2784.	3.4	70
121	Statistical Potential for Modeling and Ranking of Proteinâ€“Ligand Interactions. Journal of Chemical Information and Modeling, 2011, 51, 3078-3092.	5.4	69
122	Stability and equilibria of promiscuous aggregates in high protein milieus. Molecular BioSystems, 2007, 3, 208.	2.9	67
123	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
124	The complexed structure and antimicrobial activity of a nonâ€Îβâ€lactam inhibitor of AmpC Î²â€lactamase. Protein Science, 1999, 8, 2330-2337.	7.6	66
125	Actin Is Required for IFT Regulation in Chlamydomonas reinhardtii. Current Biology, 2014, 24, 2025-2032.	3.9	66
126	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

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127	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
128	Probing Molecular Docking in a Charged Model Binding Site. Journal of Molecular Biology, 2006, 357, 1449-1470.	4.2	61
129	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
130	The activities of drug inactive ingredients on biological targets. Science, 2020, 369, 403-413.	12.6	61
131	Discovery of Lysine-Targeted eIF4E Inhibitors through Covalent Docking. Journal of the American Chemical Society, 2020, 142, 4960-4964.	13.7	60
132	Increasing Chemical Space Coverage by Combining Empirical and Computational Fragment Screens. ACS Chemical Biology, 2014, 9, 1528-1535.	3.4	58
133	Colloidal Aggregation and the in Vitro Activity of Traditional Chinese Medicines. ACS Chemical Biology, 2015, 10, 978-988.	3.4	58
134	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
135	Muscarinic Receptors as Model Targets and Antitargets for Structure-Based Ligand Discovery. Molecular Pharmacology, 2013, 84, 528-540.	2.3	56
136	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
137	Blind Prediction of Charged Ligand Binding Affinities in a Model Binding Site. Journal of Molecular Biology, 2013, 425, 4569-4583.	4.2	53
138	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
139	An allosteric modulator binds to a conformational hub in the Î²2 adrenergic receptor. Nature Chemical Biology, 2020, 16, 749-755.	8.0	51
140	Noncovalent interaction energies in covalent complexes: TEM-1 ?-lactamase and ?-lactams. Proteins: Structure, Function and Bioinformatics, 2002, 47, 86-96.	2.6	48
141	Property-Unmatched Decoys in Docking Benchmarks. Journal of Chemical Information and Modeling, 2021, 61, 699-714.	5.4	48
142	Reverse translation of adverse event reports paves the way for de-risking preclinical off-targets. ELife, 2017, 6, .	6.0	44
143	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
144	Activity-Independent Discovery of Secondary Metabolites Using Chemical Elicitation and Cheminformatic Inference. ACS Chemical Biology, 2015, 10, 2616-2623.	3.4	43

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145	Docking and Linking of Fragments To Discover Jumonji Histone Demethylase Inhibitors. Journal of Medicinal Chemistry, 2016, 59, 1580-1598.	6.4	43
146	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
147	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
148	Prediction and validation of enzyme and transporter off-targets for metformin. Journal of Pharmacokinetics and Pharmacodynamics, 2015, 42, 463-475.	1.8	37
149	Inhibition of AmpC Î²-Lactamase through a Destabilizing Interaction in the Active Site,. Biochemistry, 2001, 40, 7992-7999.	2.5	36
150	Stable Colloidal Drug Aggregates Catch and Release Active Enzymes. ACS Chemical Biology, 2016, 11, 992-1000.	3.4	36
151	Functional analyses of AmpC Î²â€lactamase through differential stability. Protein Science, 1999, 8, 1816-1824.	7.6	34
152	The Hunt for 8-Oxoguanine Deaminase. Journal of the American Chemical Society, 2010, 132, 1762-1763.	13.7	34
153	Virtual Screening for UDP-Galactopyranose Mutase Ligands Identifies a New Class of Antimycobacterial Agents. ACS Chemical Biology, 2015, 10, 2209-2218.	3.4	34
154	Reâ€examining the role of Lys67 in class C Î²â€lactamase catalysis. Protein Science, 2009, 18, 662-669.	7.6	32
155	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
156	Small-Molecule Allosteric Modulators of the Protein Kinase PDK1 from Structure-Based Docking. Journal of Medicinal Chemistry, 2015, 58, 8285-8291.	6.4	32
157	Selectivity Challenges in Docking Screens for GPCR Targets and Antitargets. Journal of Medicinal Chemistry, 2018, 61, 6830-6845.	6.4	31
158	Prediction of enzymatic pathways by integrative pathway mapping. ELife, 2018, 7, .	6.0	30
159	Ligand Strain Energy in Large Library Docking. Journal of Chemical Information and Modeling, 2021, 61, 4331-4341.	5.4	29
160	In Vitro and In Vivo Characterization of the Alkaloid Nuciferine. PLoS ONE, 2016, 11, e0150602.	2.5	28
161	Large-Scale Identification and Analysis of Suppressive Drug Interactions. Chemistry and Biology, 2014, 21, 541-551.	6.0	27
162	Internal Structure and Preferential Protein Binding of Colloidal Aggregates. ACS Chemical Biology, 2017, 12, 282-290.	3.4	26

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163	Colloidal Drug Aggregate Stability in High Serum Conditions and Pharmacokinetic Consequence. ACS Chemical Biology, 2019, 14, 751-757.	3.4	25
164	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
165	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
166	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
167	Roles for Ordered and Bulk Solvent in Ligand Recognition and Docking in Two Related Cavities. PLoS ONE, 2013, 8, e69153.	2.5	23
168	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
169	Protein Stability Effects in Aggregate-Based Enzyme Inhibition. Journal of Medicinal Chemistry, 2019, 62, 9593-9599.	6.4	20
170	Structure-Based Design and Discovery of New M₂ Receptor Agonists. Journal of Medicinal Chemistry, 2017, 60, 9239-9250.	6.4	19
171	Colloidal Aggregators in Biochemical SARS-CoV-2 Repurposing Screens. Journal of Medicinal Chemistry, 2021, 64, 17530-17539.	6.4	19
172	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
173	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
174	Identification of Novel Smoothened Ligands Using Structure-Based Docking. PLoS ONE, 2016, 11, e0160365.	2.5	17
175	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
176	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
177	Leveraging Colloidal Aggregation for Drug-Rich Nanoparticle Formulations. Molecular Pharmaceutics, 2017, 14, 1852-1860.	4.6	16
178	Interactions of Oral Molecular Excipients with Breast Cancer Resistance Protein, BCRP. Molecular Pharmaceutics, 2020, 17, 748-756.	4.6	16
179	Thermodynamic Cycle Analysis and Inhibitor Design against Beta-Lactamaseâ€. Biochemistry, 2003, 42, 14483-14491.	2.5	14
180	No free energy lunch. Nature Biotechnology, 2007, 25, 1109-1110.	17.5	14

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181	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
182	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
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