Brian K Shoichet

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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	ZINC--a free database of commercially available compounds for virtual screening. *Journal of Chemical Information and Modeling*, **2005**, 45, 177-82	6.1	2793
195	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. *Nature*, **2020**, 583, 459-468	50.4	2142
194	Relating protein pharmacology by ligand chemistry. *Nature Biotechnology*, **2007**, 25, 197-206	44.5	1278
193	Predicting new molecular targets for known drugs. *Nature*, **2009**, 462, 175-81	50.4	1212
192	Benchmarking sets for molecular docking. *Journal of Medicinal Chemistry*, **2006**, 49, 6789-801	8.3	1023
191	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
190	Virtual screening of chemical libraries. *Nature*, **2004**, 432, 862-5	50.4	968
189	A common mechanism underlying promiscuous inhibitors from virtual and high-throughput screening. *Journal of Medicinal Chemistry*, **2002**, 45, 1712-22	8.3	924
188	Automated docking with grid-based energy evaluation. *Journal of Computational Chemistry*, **1992**, 13, 505-524	3.5	770
187	Large-scale prediction and testing of drug activity on side-effect targets. *Nature*, **2012**, 486, 361-7	50.4	623
186	Structure-based discovery of opioid analgesics with reduced side effects. *Nature*, **2016**, 537, 185-190	50.4	547
185	Prediction of protein-ligand interactions. Docking and scoring: successes and gaps. *Journal of Medicinal Chemistry*, **2006**, 49, 5851-5	8.3	542
184	A specific mechanism of nonspecific inhibition. *Journal of Medicinal Chemistry*, **2003**, 46, 4265-72	8.3	529
183	The promise and peril of chemical probes. *Nature Chemical Biology*, **2015**, 11, 536-41	11.7	523
182	The Global Phosphorylation Landscape of SARS-CoV-2 Infection. *Cell*, **2020**, 182, 685-712.e19	56.2	439
181	Identification and prediction of promiscuous aggregating inhibitors among known drugs. *Journal of Medicinal Chemistry*, **2003**, 46, 4477-86	8.3	428
180	Rapid behavior-based identification of neuroactive small molecules in the zebrafish. *Nature Chemical Biology*, **2010**, 6, 231-237	11.7	398

179	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
178	Lead discovery using molecular docking. *Current Opinion in Chemical Biology*, **2002**, 6, 439-46	9.7	355
177	Evolution of an antibiotic resistance enzyme constrained by stability and activity trade-offs. *Journal of Molecular Biology*, **2002**, 320, 85-95	6.5	355
176	Molecular docking using shape descriptors. *Journal of Computational Chemistry*, **1992**, 13, 380-397	3.5	348
175	A detergent-based assay for the detection of promiscuous inhibitors. *Nature Protocols*, **2006**, 1, 550-3	18.8	335
174	Ultra-large library docking for discovering new chemotypes. *Nature*, **2019**, 566, 224-229	50.4	309
173	Structure-Based Molecular Design. *Accounts of Chemical Research*, **1994**, 27, 117-123	24.3	297
172	A high-throughput screen for aggregation-based inhibition in a large compound library. *Journal of Medicinal Chemistry*, **2007**, 50, 2385-90	8.3	288
171	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
170	Protein docking and complementarity. *Journal of Molecular Biology*, **1991**, 221, 327-46	6.5	264
169	High-throughput assays for promiscuous inhibitors **2005**, 1, 146-8		261
168	Comparative host-coronavirus protein interaction networks reveal pan-viral disease mechanisms. *Science*, **2020**, 370,	33.3	261
167	An Aggregation Advisor for Ligand Discovery. *Journal of Medicinal Chemistry*, **2015**, 58, 7076-87	8.3	258
166	Ligand discovery from a dopamine D3 receptor homology model and crystal structure. *Nature Chemical Biology*, **2011**, 7, 769-78	11.7	250
165	Structure of the D2 dopamine receptor bound to the atypical antipsychotic drug risperidone. *Nature*, **2018**, 555, 269-273	50.4	243
164	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
163	Predicting absolute ligand binding free energies to a simple model site. *Journal of Molecular Biology*, **2007**, 371, 1118-34	6.5	234
162	Interpreting steep dose-response curves in early inhibitor discovery. *Journal of Medicinal Chemistry*, **2006**, 49, 7274-7	8.3	232

161	Kinase inhibitors: not just for kinases anymore. *Journal of Medicinal Chemistry*, **2003**, 46, 1478-83	8.3	231
160	Structure-based drug screening for G-protein-coupled receptors. *Trends in Pharmacological Sciences* , **2012**, 33, 268-72	13.2	229
159	Screening in a spirit haunted world. *Drug Discovery Today*, **2006**, 11, 607-15	8.8	228
158	Small-molecule aggregates inhibit amyloid polymerization. *Nature Chemical Biology*, **2008**, 4, 197-9	11.7	223
157	Ligand solvation in molecular docking. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 4-16	4.2	223
156	Flexible ligand docking using conformational ensembles. *Protein Science*, **1998**, 7, 938-50	6.3	217
155	Structure-based activity prediction for an enzyme of unknown function. *Nature*, **2007**, 448, 775-9	50.4	216
154	Crystal Structure of an LSD-Bound Human Serotonin Receptor. *Cell*, **2017**, 168, 377-389.e12	56.2	214
153	Rapid context-dependent ligand desolvation in molecular docking. *Journal of Chemical Information and Modeling*, **2010**, 50, 1561-73	6.1	213
152	Automated docking screens: a feasibility study. *Journal of Medicinal Chemistry*, **2009**, 52, 5712-20	8.3	213
151	Soft docking and multiple receptor conformations in virtual screening. *Journal of Medicinal Chemistry*, **2004**, 47, 5076-84	8.3	199
150	Molecular docking and ligand specificity in fragment-based inhibitor discovery. *Nature Chemical Biology*, **2009**, 5, 358-64	11.7	197
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148	Structural bases of stability-function tradeoffs in enzymes. *Journal of Molecular Biology*, **2002**, 321, 285-96	6.5	188
147	Covalent docking of large libraries for the discovery of chemical probes. *Nature Chemical Biology*, **2014**, 10, 1066-72	11.7	178
146	A model binding site for testing scoring functions in molecular docking. *Journal of Molecular Biology*, **2002**, 322, 339-55	6.5	178
145	Quantifying biogenic bias in screening libraries. *Nature Chemical Biology*, **2009**, 5, 479-83	11.7	175
144	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

143	Matching chemistry and shape in molecular docking. *Protein Engineering, Design and Selection*, **1993**, 6, 723-32	1.9	170
142	Stoichiometry and physical chemistry of promiscuous aggregate-based inhibitors. *Journal of the American Chemical Society*, **2008**, 130, 9606-12	16.4	169
141	Docking Screens for Novel Ligands Conferring New Biology. *Journal of Medicinal Chemistry*, **2016**, 59, 4103-20	8.3	166
140	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
139	Testing a flexible-receptor docking algorithm in a model binding site. *Journal of Molecular Biology*, **2004**, 337, 1161-82	6.5	164
138	Promiscuous aggregate-based inhibitors promote enzyme unfolding. *Journal of Medicinal Chemistry*, **2009**, 52, 2067-75	8.3	163
137	In silico design of novel probes for the atypical opioid receptor MRGPRX2. *Nature Chemical Biology*, **2017**, 13, 529-536	11.7	158
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135	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
134	Rescoring docking hit lists for model cavity sites: predictions and experimental testing. *Journal of Molecular Biology*, **2008**, 377, 914-34	6.5	149
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129	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
128	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
127	A SARS-CoV-2-Human Protein-Protein Interaction Map Reveals Drug Targets and Potential Drug-Repurposing **2020**,		133
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81	Stability and equilibria of promiscuous aggregates in high protein milieus. *Molecular BioSystems*, **2007**, 3, 208-13		58
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55	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
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53	Virtual Screening for UDP-Galactopyranose Mutase Ligands Identifies a New Class of Antimycobacterial Agents. *ACS Chemical Biology*, **2015**, 10, 2209-18	4.9	28
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39	Small-Molecule Allosteric Modulators of the Protein Kinase PDK1 from Structure-Based Docking. *Journal of Medicinal Chemistry*, **2015**, 58, 8285-8291	8.3	19
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