John J Irwin

List of Publications by Year in descending order

37 papers	15,021 citations	172457 29 h-index	315739 38 g-index
42 all docs	42 docs citations	42 times ranked	17166 citing authors

#	Article	IF	Citations
1	CACHE (Critical Assessment of Computational Hit-finding Experiments): A publicâ€“private partnership benchmarking initiative to enable the development of computational methods for hit-finding. Nature Reviews Chemistry, 2022, 6, 287-295.	30.2	22
2	Drug building blocks and libraries at risk in Ukraine. Science, 2022, 376, 929-929.	12.6	1
3	Property-Unmatched Decoys in Docking Benchmarks. Journal of Chemical Information and Modeling, 2021, 61, 699-714.	5.4	48
4	Fragment binding to the Nsp3 macrodomain of SARS-CoV-2 identified through crystallographic screening and computational docking. Science Advances, 2021, 7, .	10.3	100
5	Ligand Strain Energy in Large Library Docking. Journal of Chemical Information and Modeling, 2021, 61, 4331-4341.	5.4	29
6	A practical guide to large-scale docking. Nature Protocols, 2021, 16, 4799-4832.	12.0	206
7	Structures of the Ïƒ2 receptor enable docking for bioactive ligand discovery. Nature, 2021, 600, 759-764.	27.8	113
8	Docking Finds GPCR Ligands in Dark Chemical Matter. Journal of Medicinal Chemistry, 2020, 63, 613-620.	6.4	13
9	The activities of drug inactive ingredients on biological targets. Science, 2020, 369, 403-413.	12.6	61
10	ZINC20â€”A Free Ultralarge-Scale Chemical Database for Ligand Discovery. Journal of Chemical Information and Modeling, 2020, 60, 6065-6073.	5.4	321
11	Virtual discovery of melatonin receptor ligands to modulate circadian rhythms. Nature, 2020, 579, 609-614.	27.8	184
12	Discovery of Lysine-Targeted eIF4E Inhibitors through Covalent Docking. Journal of the American Chemical Society, 2020, 142, 4960-4964.	13.7	60
13	Ultra-large library docking for discovering new chemotypes. Nature, 2019, 566, 224-229.	27.8	595
14	Predicted Biological Activity of Purchasable Chemical Space. Journal of Chemical Information and Modeling, 2018, 58, 148-164.	5.4	35
15	Discovery of new GPCR ligands to illuminate new biology. Nature Chemical Biology, 2017, 13, 1143-1151.	8.0	80
16	Identification of Novel Smoothened Ligands Using Structure-Based Docking. PLoS ONE, 2016, 11, e0160365.	2.5	17
17	Docking Screens for Novel Ligands Conferring New Biology. Journal of Medicinal Chemistry, 2016, 59, 4103-4120.	6.4	218
18	ZINC 15 â€“ Ligand Discovery for Everyone. Journal of Chemical Information and Modeling, 2015, 55, 2324-2337.	5.4	2,194

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19	An Aggregation Advisor for Ligand Discovery. Journal of Medicinal Chemistry, 2015, 58, 7076-7087.	6.4	350
20	Novel compounds lowering the cellular isoform of the human prion protein in cultured human cells. Bioorganic and Medicinal Chemistry, 2014, 22, 1960-1972.	3.0	24
21	Covalent docking of large libraries for the discovery of chemical probes. Nature Chemical Biology, 2014, 10, 1066-1072.	8.0	225
22	Ligand Pose and Orientational Sampling in Molecular Docking. PLoS ONE, 2013, 8, e75992.	2.5	139
23	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
24	ZINC: A Free Tool to Discover Chemistry for Biology. Journal of Chemical Information and Modeling, 2012, 52, 1757-1768.	5.4	1,985
25	Chemical informatics and target identification in a zebrafish phenotypic screen. Nature Chemical Biology, 2012, 8, 144-146.	8.0	113
26	Structure-Based Discovery of A_{2A}Adenosine Receptor Ligands. Journal of Medicinal Chemistry, 2010, 53, 3748-3755.	6.4	212
27	Predicting new molecular targets for known drugs. Nature, 2009, 462, 175-181.	27.8	1,474
28	Quantifying biogenic bias in screening libraries. Nature Chemical Biology, 2009, 5, 479-483.	8.0	198
29	Staring off into chemical space. Nature Chemical Biology, 2009, 5, 536-537.	8.0	10
30	Automated Docking Screens: A Feasibility Study. Journal of Medicinal Chemistry, 2009, 52, 5712-5720.	6.4	245
31	Community benchmarks for virtual screening. Journal of Computer-Aided Molecular Design, 2008, 22, 193-199.	2.9	154
32	Quantifying the Relationships among Drug Classes. Journal of Chemical Information and Modeling, 2008, 48, 755-765.	5.4	160
33	Relating protein pharmacology by ligand chemistry. Nature Biotechnology, 2007, 25, 197-206.	17.5	1,722
34	How good is your screening library?. Current Opinion in Chemical Biology, 2006, 10, 352-356.	6.1	38
35	Software Review:â€‰ ChemOffice 2005 Pro by CambridgeSoft. Journal of Chemical Information and Modeling, 2005, 45, 1468-1469.	5.4	5
36	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

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37	Virtual Screening against Metalloenzymes for Inhibitors and Substratesâ€. Biochemistry, 2005, 44, 12316-12328.	2.5	125