John P Overington

List of Publications by Year in descending order

106 papers	22,017 citations	50276 46 h-index	30922 102 g-index
111 all docs	111 docs citations	111 times ranked	28761 citing authors

#	Article	IF	Citations
1	How many drug targets are there?. Nature Reviews Drug Discovery, 2006, 5, 993-996.	46.4	3,073
2	ChEMBL: a large-scale bioactivity database for drug discovery. Nucleic Acids Research, 2012, 40, D1100-D1107.	14.5	3,028
3	The ChEMBL database in 2017. Nucleic Acids Research, 2017, 45, D945-D954.	14.5	1,718
4	A comprehensive map of molecular drug targets. Nature Reviews Drug Discovery, 2017, 16, 19-34.	46.4	1,608
5	The ChEMBL bioactivity database: an update. Nucleic Acids Research, 2014, 42, D1083-D1090.	14.5	1,283
6	An atlas of genetic influences on human blood metabolites. Nature Genetics, 2014, 46, 543-550.	21.4	1,084
7	The genome of the blood fluke Schistosoma mansoni. Nature, 2009, 460, 352-358.	27.8	945
8	The promise and peril of chemical probes. Nature Chemical Biology, 2015, 11, 536-541.	8.0	698
9	X-ray analysis of HIV-1 proteinase at 2.7 Ã... resolution confirms structural homology among retroviral enzymes. Nature, 1989, 342, 299-302.	27.8	477
10	Can we rationally design promiscuous drugs?. Current Opinion in Structural Biology, 2006, 16, 127-136.	5.7	472
11	HOMSTRAD: A database of protein structure alignments for homologous families. Protein Science, 1998, 7, 2469-2471.	7.6	461
12	ChEMBL web services: streamlining access to drug discovery data and utilities. Nucleic Acids Research, 2015, 43, W612-W620.	14.5	437
13	The druggable genome and support for target identification and validation in drug development. Science Translational Medicine, 2017, 9, .	12.4	437
14	Probing the links between in vitro potency, ADMET and physicochemical parameters. Nature Reviews Drug Discovery, 2011, 10, 197-208.	46.4	409
15	JOY: protein sequence-structure representation and analysis.. Bioinformatics, 1998, 14, 617-623.	4.1	384
16	Comprehensive characterization of the Published Kinase Inhibitor Set. Nature Biotechnology, 2016, 34, 95-103.	17.5	289
17	A Structural Basis for Sequence Comparisons. Journal of Molecular Biology, 1993, 233, 716-738.	4.2	286
18	Genomic-scale prioritization of drug targets: the TDR Targets database. Nature Reviews Drug Discovery, 2008, 7, 900-907.	46.4	282

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19	Derivation of rules for comparative protein modeling from a database of protein structure alignments. Protein Science, 1994, 3, 1582-1596.	7.6	275
20	PSICQUIC and PSISCORE: accessing and scoring molecular interactions. Nature Methods, 2011, 8, 528-529.	19.0	274
21	Unexplored therapeutic opportunities in the human genome. Nature Reviews Drug Discovery, 2018, 17, 317-332.	46.4	263
22	Knowledge-based protein modelling and design. FEBS Journal, 1988, 172, 513-520.	0.2	236
23	Alignment and Searching for Common Protein Folds Using a Data Bank of Structural Templates. Journal of Molecular Biology, 1993, 231, 735-752.	4.2	174
24	SureChEMBL: a large-scale, chemically annotated patent document database. Nucleic Acids Research, 2016, 44, D1220-D1228.	14.5	156
25	From comparisons of protein sequences and structures to protein modelling and design. Trends in Biochemical Sciences, 1990, 15, 235-240.	7.5	149
26	Modeling Î±â€helical transmembrane domains: The calculation and use of substitution tables for lipidâ€facing residues. Protein Science, 1993, 2, 55-70.	7.6	143
27	UniChem: a unified chemical structure cross-referencing and identifier tracking system. Journal of Cheminformatics, 2013, 5, 3.	6.1	133
28	Drug Target Commons: A Community Effort to Build a Consensus Knowledge Base for Drug-Target Interactions. Cell Chemical Biology, 2018, 25, 224-229.e2.	5.2	124
29	Fragment Ranking in Modelling of Protein Structure. Journal of Molecular Biology, 1993, 229, 194-220.	4.2	119
30	Activity, assay and target data curation and quality in the ChEMBL database. Journal of Computer-Aided Molecular Design, 2015, 29, 885-896.	2.9	118
31	Improving the odds of drug development success through human genomics: modelling study. Scientific Reports, 2019, 9, 18911.	3.3	112
32	Ligand efficiency indices for an effective mapping of chemico-biological space: the concept of an atlas-like representation. Drug Discovery Today, 2010, 15, 804-811.	6.4	102
33	Improved large-scale prediction of growth inhibition patterns using the NCI60 cancer cell line panel. Bioinformatics, 2016, 32, 85-95.	4.1	95
34	PCSK9 monoclonal antibodies for the primary and secondary prevention of cardiovascular disease. The Cochrane Library, 2017, 4, CD011748.	2.8	93
35	Computational and Practical Aspects of Drug Repositioning. Assay and Drug Development Technologies, 2015, 13, 299-306.	1.2	89
36	Comparative modelling of major house dust mite allergen Der p I: structure validation using an extended environmental amino acid propensity table. Protein Engineering, Design and Selection, 1994, 7, 869-894.	2.1	82

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37	Minimum information about a bioactive entity (MIABE). Nature Reviews Drug Discovery, 2011, 10, 661-669.	46.4	80
38	Chemical, Target, and Bioactive Properties of Allosteric Modulation. PLoS Computational Biology, 2014, 10, e1003559.	3.2	75
39	Benchmarking of protein descriptor sets in proteochemometric modeling (part 2): modeling performance of 13 amino acid descriptor sets. Journal of Cheminformatics, 2013, 5, 42.	6.1	73
40	Open Source Drug Discovery: Highly Potent Antimalarial Compounds Derived from the Tres Cantos Arylpyrroles. ACS Central Science, 2016, 2, 687-701.	11.3	68
41	The prediction and orientation of Î±-helices from sequence alignments: the combined use of environment-dependent substitution tables, Fourier transform methods and helix capping rules. Protein Engineering, Design and Selection, 1994, 7, 645-653.	2.1	58
42	Antibody informatics for drug discovery. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 2002-2015.	2.3	58
43	Artificial intelligence, drug repurposing and peer review. Nature Biotechnology, 2020, 38, 1127-1131.	17.5	56
44	Molecular recognition in protein families: A database of aligned three-dimensional structures of related proteins. Biochemical Society Transactions, 1993, 21, 597-604.	3.4	53
45	Target Prediction for an Open Access Set of Compounds Active against Mycobacterium tuberculosis. PLoS Computational Biology, 2013, 9, e1003253.	3.2	51
46	Unprecedently Large-Scale Kinase Inhibitor Set Enabling the Accurate Prediction of Compoundâ€“Kinase Activities: A Way toward Selective Promiscuity by Design?. Journal of Chemical Information and Modeling, 2016, 56, 1654-1675.	5.4	50
47	Nicastrin, a presenilin-interacting protein, contains an aminopeptidase/transferrin receptor superfamily domain. Trends in Biochemical Sciences, 2001, 26, 213-214.	7.5	49
48	[34] Discrimination of common protein folds: Application of protein structure to sequence/structure comparisons. Methods in Enzymology, 1996, 266, 575-598.	1.0	46
49	Chemical databases: curation or integration by user-defined equivalence?. Drug Discovery Today: Technologies, 2015, 14, 17-24.	4.0	43
50	Comparison of three-dimensional structures of homologous proteins. Current Opinion in Structural Biology, 1992, 2, 394-401.	5.7	42
51	The ChEMBL database: a taster for medicinal chemists. Future Medicinal Chemistry, 2014, 6, 361-364.	2.3	42
52	PDBLIG:Â Classification of Small Molecular Protein Binding in the Protein Data Bank. Journal of Medicinal Chemistry, 2004, 47, 3807-3816.	6.4	41
53	Global Analysis of Small Molecule Binding to Related Protein Targets. PLoS Computational Biology, 2012, 8, e1002333.	3.2	41
54	Mycobacterial Dihydrofolate Reductase Inhibitors Identified Using Chemogenomic Methods and In Vitro Validation. PLoS ONE, 2015, 10, e0121492.	2.5	40

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55	diXa: a data infrastructure for chemical safety assessment. Bioinformatics, 2015, 31, 1505-1507.	4.1	40
56	The relationship between target-class and the physicochemical properties of antibacterial drugs. Bioorganic and Medicinal Chemistry, 2015, 23, 5218-5224.	3.0	40
57	Release of 50 new, drug-like compounds and their computational target predictions for open source anti-tubercular drug discovery. PLoS ONE, 2015, 10, e0142293.	2.5	38
58	Synthesis of Macrocyclic, Potential Protease Inhibitors Using a Generic Scaffold. Journal of Organic Chemistry, 2002, 67, 4882-4892.	3.2	33
59	Structural and Functional View of Polypharmacology. Scientific Reports, 2017, 7, 10102.	3.3	33
60	Collation and data-mining of literature bioactivity data for drug discovery. Biochemical Society Transactions, 2011, 39, 1365-1370.	3.4	31
61	Annotating Human Pâ€Glycoprotein Bioassay Data. Molecular Informatics, 2012, 31, 599-609.	2.5	30
62	UniChem: extension of InChI-based compound mapping to salt, connectivity and stereochemistry layers. Journal of Cheminformatics, 2014, 6, 43.	6.1	28
63	A drug target slim: using gene ontology and gene ontology annotations to navigate protein-ligand target space in ChEMBL. Journal of Biomedical Semantics, 2016, 7, 59.	1.6	27
64	Repurposing Vandetanib plus Everolimus for the Treatment ofACVR1-Mutant Diffuse Intrinsic Pontine Glioma. Cancer Discovery, 2022, 12, 416-431.	9.4	25
65	Design of Selective Thrombin Inhibitors Based on the (R)-Phe-Pro-Arg Sequence. Journal of Medicinal Chemistry, 2002, 45, 2432-2453.	6.4	22
66	Prioritizing the proteome: identifying pharmaceutically relevant targets. Drug Discovery Today, 2002, 7, 516-521.	6.4	22
67	Target Identification of Mycobacterium tuberculosis Phenotypic Hits Using a Concerted Chemogenomic, Biophysical, and Structural Approach. Frontiers in Pharmacology, 2017, 8, 681.	3.5	22
68	Cheminformatics. Communications of the ACM, 2012, 55, 65-75.	4.5	21
69	Role of open chemical data in aiding drug discovery and design. Future Medicinal Chemistry, 2010, 2, 903-907.	2.3	20
70	The EBI enzyme portal. Nucleic Acids Research, 2013, 41, D773-D780.	14.5	19
71	Chemogenomics Approaches for Receptor Deorphanization and Extensions of the Chemogenomics Concept to Phenotypic Space. Current Topics in Medicinal Chemistry, 2011, 11, 1964-1977.	2.1	18
72	A ligand's-eye view of protein similarity. Nature Methods, 2013, 10, 116-117.	19.0	18

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73	myChEMBL: a virtual machine implementation of open data and cheminformatics tools. Bioinformatics, 2014, 30, 298-300.	4.1	18
74	A large-scale crop protection bioassay data set. Scientific Data, 2015, 2, 150032.	5.3	18
75	Identification of Allosteric Modulators of Metabotropic Glutamate 7 Receptor Using Proteochemometric Modeling. Journal of Chemical Information and Modeling, 2017, 57, 2976-2985.	5.4	18
76	Insights into protein function through large-scale computational analysis of sequence and structure. Trends in Biotechnology, 2001, 19, S61-S66.	9.3	17
77	Setting Our Sights on Infectious Diseases. ACS Infectious Diseases, 2020, 6, 3-13.	3.8	17
78	Insights into protein function through large-scale computational analysis of sequence and structure. Trends in Biotechnology, 2001, 19, 61-66.	9.3	16
79	Protein sequence analysis in silico: application of structure-based bioinformatics to genomic initiatives. Current Opinion in Pharmacology, 2002, 2, 574-580.	3.5	16
80	Scientific Lenses to Support Multiple Views over Linked Chemistry Data. Lecture Notes in Computer Science, 2014, , 98-113.	1.3	16
81	Rapid Analysis of Pharmacology for Infectious Diseases. Current Topics in Medicinal Chemistry, 2011, 11, 1292-1300.	2.1	15
82	Mapping small molecule binding data to structural domains. BMC Bioinformatics, 2012, 13, S11.	2.6	14
83	Classification and analysis of a large collection of in vivo bioassay descriptions. PLoS Computational Biology, 2017, 13, e1005641.	3.2	14
84	Open data for drug discovery: learning from the biological community. Future Medicinal Chemistry, 2012, 4, 1865-1867.	2.3	13
85	ADME SARfari: comparative genomics of drug metabolizing systems. Bioinformatics, 2015, 31, 1695-1697.	4.1	12
86	MyChEMBL: A Virtual Platform for Distributing Cheminformatics Tools and Open Data. Challenges, 2014, 5, 334-337.	1.7	11
87	A document classifier for medicinal chemistry publications trained on the ChEMBL corpus. Journal of Cheminformatics, 2014, 6, 40.	6.1	11
88	PPDMsâ€"a resource for mapping small molecule bioactivities from ChEMBL to Pfam-A protein domains. Bioinformatics, 2015, 31, 776-778.	4.1	11
89	Rational design of non-resistant targeted cancer therapies. Scientific Reports, 2017, 7, 46632.	3.3	11
90	Protein Three-Dimensional Structural Databases: Domains, Structurally Aligned Homologues and Superfamilies. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 1168-1177.	2.5	6

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91	The functional therapeutic chemical classification system. Bioinformatics, 2014, 30, 876-883.	4.1	6
92	The Molecular Basis of Predicting Druggability. , 0, , 1315-1334.		5
93	Brain: biomedical knowledge manipulation. Bioinformatics, 2013, 29, 1238-1239.	4.1	5
94	Transporter assays and assay ontologies: useful tools for drug discovery. Drug Discovery Today: Technologies, 2014, 12, e47-e54.	4.0	4
95	Modelling of the lignin peroxidase LIII of Phlebia radiata: use of a sequence template generated from a 3-D structure. Protein Engineering, Design and Selection, 1993, 6, 177-182.	2.1	3
96	Chapter 28. Recent development in cheminformatics and chemogenomics. Annual Reports in Medicinal Chemistry, 2003, 38, 285-294.	0.9	3
97	Knowledge-Based Protein Modelling: Human Plasma Kallikrein and Human Neutrophil Defensin. , 1990, , 567-574.		3
98	Chapter 19. Expanding and exploring cellular pathways for novel drug targets. Annual Reports in Medicinal Chemistry, 2002, 37, 187-196.	0.9	2
99	Pleiotropic Effects of Statins. Annual Reports in Medicinal Chemistry, 2004, 39, 239-258.	0.9	2
100	ChEMBL Beaker: A Lightweight Web Framework Providing Robust and Extensible Cheminformatics Services. Challenges, 2014, 5, 444-449.	1.7	2
101	Towards predictive resistance models for agrochemicals by combining chemical and protein similarity via proteochemometric modelling. Journal of Chemical Biology, 2014, 7, 119-123.	2.2	2
102	Comparison of three-dimensional structures of homologous proteins. Current Biology, 1992, 2, 376.	3.9	1
103	The comparison of structures and sequences: alignment, searching and the detection of common folds. , 1994, , .		1
104	Symposium 1: Structure and engineering of proteins: New developments. Fresenius' Journal of Analytical Chemistry, 1990, 337, 1-3.	1.5	0
105	New open drug activity data at EBI. Chemistry Central Journal, 2009, 3, .	2.6	0
106	Knowledge-Based Protein Modeling and the Design of Novel Molecules. , 1990, , 209-227.		0