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	Repurposing Vandetanib plus Everolimus for the Treatment ofACVR1-Mutant Diffuse Intrinsic Pontine Glioma. Cancer Discovery, 2022, 12, 416-431.	9.4	25
2	Setting Our Sights on Infectious Diseases. ACS Infectious Diseases, 2020, 6, 3-13.	3.8	17
3	Artificial intelligence, drug repurposing and peer review. Nature Biotechnology, 2020, 38, 1127-1131.	17.5	56
4	Improving the odds of drug development success through human genomics: modelling study. Scientific Reports, 2019, 9, 18911.	3.3	112
5	Unexplored therapeutic opportunities in the human genome. Nature Reviews Drug Discovery, 2018, 17, 317-332.	46.4	263
6	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
7	Rational design of non-resistant targeted cancer therapies. Scientific Reports, 2017, 7, 46632.	3.3	11
8	PCSK9 monoclonal antibodies for the primary and secondary prevention of cardiovascular disease. The Cochrane Library, 2017, 4, CD011748.	2.8	93
9	A comprehensive map of molecular drug targets. Nature Reviews Drug Discovery, 2017, 16, 19-34.	46.4	1,608
10	The druggable genome and support for target identification and validation in drug development. Science Translational Medicine, 2017, 9, .	12.4	437
11	Structural and Functional View of Polypharmacology. Scientific Reports, 2017, 7, 10102.	3.3	33
12	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
13	The ChEMBL database in 2017. Nucleic Acids Research, 2017, 45, D945-D954.	14.5	1,718
14	Target Identification of Mycobacterium tuberculosis Phenotypic Hits Using a Concerted Chemogenomic, Biophysical, and Structural Approach. Frontiers in Pharmacology, 2017, 8, 681.	3.5	22
15	Classification and analysis of a large collection of in vivo bioassay descriptions. PLoS Computational Biology, 2017, 13, e1005641.	3.2	14
16	Improved large-scale prediction of growth inhibition patterns using the NCI60 cancer cell line panel. Bioinformatics, 2016, 32, 85-95.	4.1	95
17	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
18	Open Source Drug Discovery: Highly Potent Antimalarial Compounds Derived from the Tres Cantos Arylpyrroles. ACS Central Science, 2016, 2, 687-701.	11.3	68

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19	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
20	SureChEMBL: a large-scale, chemically annotated patent document database. Nucleic Acids Research, 2016, 44, D1220-D1228.	14.5	156
21	Comprehensive characterization of the Published Kinase Inhibitor Set. Nature Biotechnology, 2016, 34, 95-103.	17.5	289
22	A large-scale crop protection bioassay data set. Scientific Data, 2015, 2, 150032.	5.3	18
23	Mycobacterial Dihydrofolate Reductase Inhibitors Identified Using Chemogenomic Methods and In Vitro Validation. PLoS ONE, 2015, 10, e0121492.	2.5	40
24	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
25	ChEMBL web services: streamlining access to drug discovery data and utilities. Nucleic Acids Research, 2015, 43, W612-W620.	14.5	437
26	diXa: a data infrastructure for chemical safety assessment. Bioinformatics, 2015, 31, 1505-1507.	4.1	40
27	ADME SARfari: comparative genomics of drug metabolizing systems. Bioinformatics, 2015, 31, 1695-1697.	4.1	12
28	The promise and peril of chemical probes. Nature Chemical Biology, 2015, 11, 536-541.	8.0	698
29	The relationship between target-class and the physicochemical properties of antibacterial drugs. Bioorganic and Medicinal Chemistry, 2015, 23, 5218-5224.	3.0	40
30	PPDMsâ€"a resource for mapping small molecule bioactivities from ChEMBL to Pfam-A protein domains. Bioinformatics, 2015, 31, 776-778.	4.1	11
31	Chemical databases: curation or integration by user-defined equivalence?. Drug Discovery Today: Technologies, 2015, 14, 17-24.	4.0	43
32	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
33	Computational and Practical Aspects of Drug Repositioning. Assay and Drug Development Technologies, 2015, 13, 299-306.	1.2	89
34	The ChEMBL bioactivity database: an update. Nucleic Acids Research, 2014, 42, D1083-D1090.	14.5	1,283
35	Chemical, Target, and Bioactive Properties of Allosteric Modulation. PLoS Computational Biology, 2014, 10, e1003559.	3.2	75
36	ChEMBL Beaker: A Lightweight Web Framework Providing Robust and Extensible Cheminformatics Services. Challenges, 2014, 5, 444-449.	1.7	2

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37	The ChEMBL database: a taster for medicinal chemists. Future Medicinal Chemistry, 2014, 6, 361-364.	2.3	42
38	The functional therapeutic chemical classification system. Bioinformatics, 2014, 30, 876-883.	4.1	6
39	myChEMBL: a virtual machine implementation of open data and cheminformatics tools. Bioinformatics, 2014, 30, 298-300.	4.1	18
40	MyChEMBL: A Virtual Platform for Distributing Cheminformatics Tools and Open Data. Challenges, 2014, 5, 334-337.	1.7	11
41	An atlas of genetic influences on human blood metabolites. Nature Genetics, 2014, 46, 543-550.	21.4	1,084
42	A document classifier for medicinal chemistry publications trained on the ChEMBL corpus. Journal of Cheminformatics, 2014, 6, 40.	6.1	11
43	UniChem: extension of InChI-based compound mapping to salt, connectivity and stereochemistry layers. Journal of Cheminformatics, 2014, 6, 43.	6.1	28
44	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
45	Antibody informatics for drug discovery. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 2002-2015.	2.3	58
46	Transporter assays and assay ontologies: useful tools for drug discovery. Drug Discovery Today: Technologies, 2014, 12, e47-e54.	4.0	4
47	Scientific Lenses to Support Multiple Views over Linked Chemistry Data. Lecture Notes in Computer Science, 2014, , 98-113.	1.3	16
48	UniChem: a unified chemical structure cross-referencing and identifier tracking system. Journal of Cheminformatics, 2013, 5, 3.	6.1	133
49	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
50	A ligand's-eye view of protein similarity. Nature Methods, 2013, 10, 116-117.	19.0	18
51	Brain: biomedical knowledge manipulation. Bioinformatics, 2013, 29, 1238-1239.	4.1	5
52	The EBI enzyme portal. Nucleic Acids Research, 2013, 41, D773-D780.	14.5	19
53	Target Prediction for an Open Access Set of Compounds Active against Mycobacterium tuberculosis. PLoS Computational Biology, 2013, 9, e1003253.	3.2	51
54	Open data for drug discovery: learning from the biological community. Future Medicinal Chemistry, 2012, 4, 1865-1867.	2.3	13

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55	Cheminformatics. Communications of the ACM, 2012, 55, 65-75.	4.5	21
56	Annotating Human Pâ€Glycoprotein Bioassay Data. Molecular Informatics, 2012, 31, 599-609.	2.5	30
57	Mapping small molecule binding data to structural domains. BMC Bioinformatics, 2012, 13, S11.	2.6	14
58	Global Analysis of Small Molecule Binding to Related Protein Targets. PLoS Computational Biology, 2012, 8, e1002333.	3.2	41
59	ChEMBL: a large-scale bioactivity database for drug discovery. Nucleic Acids Research, 2012, 40, D1100-D1107.	14.5	3,028
60	PSICQUIC and PSISCORE: accessing and scoring molecular interactions. Nature Methods, 2011, 8, 528-529.	19.0	274
61	Minimum information about a bioactive entity (MIABE). Nature Reviews Drug Discovery, 2011, 10, 661-669.	46.4	80
62	Rapid Analysis of Pharmacology for Infectious Diseases. Current Topics in Medicinal Chemistry, 2011, 11, 1292-1300.	2.1	15
63	Collation and data-mining of literature bioactivity data for drug discovery. Biochemical Society Transactions, 2011, 39, 1365-1370.	3.4	31
64	Probing the links between in vitro potency, ADMET and physicochemical parameters. Nature Reviews Drug Discovery, 2011, 10, 197-208.	46.4	409
65	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
66	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
67	Role of open chemical data in aiding drug discovery and design. Future Medicinal Chemistry, 2010, 2, 903-907.	2.3	20
68	New open drug activity data at EBI. Chemistry Central Journal, 2009, 3, .	2.6	0
69	The genome of the blood fluke Schistosoma mansoni. Nature, 2009, 460, 352-358.	27.8	945
70	Genomic-scale prioritization of drug targets: the TDR Targets database. Nature Reviews Drug Discovery, 2008, 7, 900-907.	46.4	282
71	How many drug targets are there?. Nature Reviews Drug Discovery, 2006, 5, 993-996.	46.4	3,073
72	Can we rationally design promiscuous drugs?. Current Opinion in Structural Biology, 2006, 16, 127-136.	5.7	472

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73	Pleiotropic Effects of Statins. Annual Reports in Medicinal Chemistry, 2004, 39, 239-258.	0.9	2
74	PDBLIG:Â Classification of Small Molecular Protein Binding in the Protein Data Bank. Journal of Medicinal Chemistry, 2004, 47, 3807-3816.	6.4	41
75	Chapter 28. Recent development in cheminformatics and chemogenomics. Annual Reports in Medicinal Chemistry, 2003, 38, 285-294.	0.9	3
76	Chapter 19. Expanding and exploring cellular pathways for novel drug targets. Annual Reports in Medicinal Chemistry, 2002, 37, 187-196.	0.9	2
77	Synthesis of Macrocyclic, Potential Protease Inhibitors Using a Generic Scaffold. Journal of Organic Chemistry, 2002, 67, 4882-4892.	3.2	33
78	Design of Selective Thrombin Inhibitors Based on the (R)-Phe-Pro-Arg Sequence. Journal of Medicinal Chemistry, 2002, 45, 2432-2453.	6.4	22
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	Prioritizing the proteome: identifying pharmaceutically relevant targets. Drug Discovery Today, 2002, 7, 516-521.	6.4	22
81	Insights into protein function through large-scale computational analysis of sequence and structure. Trends in Biotechnology, 2001, 19, 61-66.	9.3	16
82	Insights into protein function through large-scale computational analysis of sequence and structure. Trends in Biotechnology, 2001, 19, S61-S66.	9.3	17
83	Nicastrin, a presenilin-interacting protein, contains an aminopeptidase/transferrin receptor superfamily domain. Trends in Biochemical Sciences, 2001, 26, 213-214.	7.5	49
84	HOMSTRAD: A database of protein structure alignments for homologous families. Protein Science, 1998, 7, 2469-2471.	7.6	461
85	Protein Three-Dimensional Structural Databases: Domains, Structurally Aligned Homologues and Superfamilies. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 1168-1177.	2.5	6
86	JOY: protein sequence-structure representation and analysis.. Bioinformatics, 1998, 14, 617-623.	4.1	384
87	[34] Discrimination of common protein folds: Application of protein structure to sequence/structure comparisons. Methods in Enzymology, 1996, 266, 575-598.	1.0	46
88	Derivation of rules for comparative protein modeling from a database of protein structure alignments. Protein Science, 1994, 3, 1582-1596.	7.6	275
89	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
90	The comparison of structures and sequences: alignment, searching and the detection of common folds. , 1994, , .		1

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91	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
92	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
93	Fragment Ranking in Modelling of Protein Structure. Journal of Molecular Biology, 1993, 229, 194-220.	4.2	119
94	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
95	A Structural Basis for Sequence Comparisons. Journal of Molecular Biology, 1993, 233, 716-738.	4.2	286
96	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
97	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
98	Comparison of three-dimensional structures of homologous proteins. Current Opinion in Structural Biology, 1992, 2, 394-401.	5.7	42
99	Comparison of three-dimensional structures of homologous proteins. Current Biology, 1992, 2, 376.	3.9	1
100	Symposium 1: Structure and engineering of proteins: New developments. Fresenius' Journal of Analytical Chemistry, 1990, 337, 1-3.	1.5	0
101	From comparisons of protein sequences and structures to protein modelling and design. Trends in Biochemical Sciences, 1990, 15, 235-240.	7.5	149
102	Knowledge-Based Protein Modelling: Human Plasma Kallikrein and Human Neutrophil Defensin. , 1990, , 567-574.		3
103	Knowledge-Based Protein Modeling and the Design of Novel Molecules. , 1990, , 209-227.		0
104	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
105	Knowledge-based protein modelling and design. FEBS Journal, 1988, 172, 513-520.	0.2	236
106	The Molecular Basis of Predicting Druggability. , 0, , 1315-1334.		5