Anna Gaulton

List of Publications by Year
in descending order

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49 papers	13,530 citations	186265 28 h-index	223800 46 g-index
57 all docs	57 docs citations	57 times ranked	18232 citing authors

#	Article	IF	Citations
1	ChEMBL: a large-scale bioactivity database for drug discovery. Nucleic Acids Research, 2012, 40, D1100-D1107.	14.5	3,028
2	The ChEMBL database in 2017. Nucleic Acids Research, 2017, 45, D945-D954.	14.5	1,718
3	A comprehensive map of molecular drug targets. Nature Reviews Drug Discovery, 2017, 16, 19-34.	46.4	1,608
4	The ChEMBL bioactivity database: an update. Nucleic Acids Research, 2014, 42, D1083-D1090.	14.5	1,283
5	ChEMBL: towards direct deposition of bioassay data. Nucleic Acids Research, 2019, 47, D930-D940.	14.5	1,212
6	The Global Phosphorylation Landscape of SARS-CoV-2 Infection. Cell, 2020, 182, 685-712.e19.	28.9	825
7	ChEMBL web services: streamlining access to drug discovery data and utilities. Nucleic Acids Research, 2015, 43, W612-W620.	14.5	437
8	The druggable genome and support for target identification and validation in drug development. Science Translational Medicine, 2017, 9, .	12.4	437
9	Open Targets: a platform for therapeutic target identification and validation. Nucleic Acids Research, 2017, 45, D985-D994.	14.5	355
10	PSICQUIC and PSISCORE: accessing and scoring molecular interactions. Nature Methods, 2011, 8, 528-529.	19.0	274
11	Pharos: Collating protein information to shed light on the druggable genome. Nucleic Acids Research, 2017, 45, D995-D1002.	14.5	271
12	Unexplored therapeutic opportunities in the human genome. Nature Reviews Drug Discovery, 2018, 17, 317-332.	46.4	263
13	The EBI RDF platform: linked open data for the life sciences. Bioinformatics, 2014, 30, 1338-1339.	4.1	190
14	An open source chemical structure curation pipeline using RDKit. Journal of Cheminformatics, 2020, 12, 51.	6.1	166
15	SureChEMBL: a large-scale, chemically annotated patent document database. Nucleic Acids Research, 2016, 44, D1220-D1228.	14.5	156
16	UniChem: a unified chemical structure cross-referencing and identifier tracking system. Journal of Cheminformatics, 2013, 5, 3.	6.1	133
17	Actionable druggable genome-wide Mendelian randomization identifies repurposing opportunities for COVID-19. Nature Medicine, 2021, 27, 668-676.	30.7	120
18	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

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19	Improving the odds of drug development success through human genomics: modelling study. Scientific Reports, 2019, 9, 18911.	3.3	112
20	The complex portal - an encyclopaedia of macromolecular complexes. Nucleic Acids Research, 2015, 43, D479-D484.	14.5	100
21	Large scale comparison of QSAR and conformal prediction methods and their applications in drug discovery. Journal of Cheminformatics, 2019, 11, 4.	6.1	93
22	Minimum information about a bioactive entity (MIABE). Nature Reviews Drug Discovery, 2011, 10, 661-669.	46.4	80
23	Chemical, Target, and Bioactive Properties of Allosteric Modulation. PLoS Computational Biology, 2014, 10, e1003559.	3.2	75
24	Visualizing the drug target landscape. Drug Discovery Today, 2010, 15, 3-15.	6.4	50
25	Target-Based Evaluation of â€œDrug-Likeâ€•Properties and Ligand Efficiencies. Journal of Medicinal Chemistry, 2021, 64, 7210-7230.	6.4	46
26	Chemical databases: curation or integration by user-defined equivalence?. Drug Discovery Today: Technologies, 2015, 14, 17-24.	4.0	43
27	Bioinformatics approaches for the classification of G-protein-coupled receptors. Current Opinion in Pharmacology, 2003, 3, 114-120.	3.5	38
28	Collation and data-mining of literature bioactivity data for drug discovery. Biochemical Society Transactions, 2011, 39, 1365-1370.	3.4	31
29	UniChem: extension of InChI-based compound mapping to salt, connectivity and stereochemistry layers. Journal of Cheminformatics, 2014, 6, 43.	6.1	28
30	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
31	Using ChEMBL web services for building applications and data processing workflows relevant to drug discovery. Expert Opinion on Drug Discovery, 2017, 12, 757-767.	5.0	24
32	Role of open chemical data in aiding drug discovery and design. Future Medicinal Chemistry, 2010, 2, 903-907.	2.3	20
33	Managing expectations: assessment of chemistry databases generated by automated extraction of chemical structures from patents. Journal of Cheminformatics, 2015, 7, 49.	6.1	19
34	A large-scale crop protection bioassay data set. Scientific Data, 2015, 2, 150032.	5.3	18
35	Drug target central. Expert Opinion on Drug Discovery, 2009, 4, 857-872.	5.0	16
36	Scientific Lenses to Support Multiple Views over Linked Chemistry Data. Lecture Notes in Computer Science, 2014, , 98-113.	1.3	16

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37	Drug Safety Data Curation and Modeling in ChEMBL: Boxed Warnings and Withdrawn Drugs. Chemical Research in Toxicology, 2021, 34, 385-395.	3.3	15
38	Validation of lipid-related therapeutic targets for coronary heart disease prevention using human genetics. Nature Communications, 2021, 12, 6120.	12.8	13
39	Functional assignment of MAPK phosphatase domains. Proteins: Structure, Function and Bioinformatics, 2007, 69, 19-31.	2.6	12
40	Motif3D: relating protein sequence motifs to 3D structure. Nucleic Acids Research, 2003, 31, 3333-3336.	14.5	11
41	PPDMsâ€"a resource for mapping small molecule bioactivities from ChEMBL to Pfam-A protein domains. Bioinformatics, 2015, 31, 776-778.	4.1	11
42	A large-scale dataset of in vivo pharmacology assay results. Scientific Data, 2018, 5, 180230.	5.3	8
43	Transporter taxonomy â€" a comparison of different transport protein classification schemes. Drug Discovery Today: Technologies, 2014, 12, e37-e46.	4.0	7
44	The Molecular Basis of Predicting Druggability. , 0, , 1315-1334.		5
45	Transporter assays and assay ontologies: useful tools for drug discovery. Drug Discovery Today: Technologies, 2014, 12, e47-e54.	4.0	4
46	Reply to â€œMissed opportunities in large scale comparison of QSAR and conformal prediction methods and their applications in drug discoveryâ€• Journal of Cheminformatics, 2019, 11, 64.	6.1	4
47	The PRINTS protein fingerprint database: functional and evolutionary applications. , 2006, , .		2
48	The PRINTS protein fingerprint database: functional and evolutionary applications. , 2005, , .		1
49	Shouldn't enantiomeric purity be included in the 'minimum information about a bioactive entity? Response from the MIABE group. Nature Reviews Drug Discovery, 2012, 11, 730-730.	46.4	0