Anna Gaulton

List of Publications by Year
in descending order

49 papers	13,530 citations	185998 28 h-index	223531 46 g-index
57 all docs	57 docs citations	57 times ranked	18232 citing authors

#	Article	IF	Citations
1	Drug Safety Data Curation and Modeling in ChEMBL: Boxed Warnings and Withdrawn Drugs. Chemical Research in Toxicology, 2021, 34, 385-395.	1.7	15
2	Actionable druggable genome-wide Mendelian randomization identifies repurposing opportunities for COVID-19. Nature Medicine, 2021, 27, 668-676.	15.2	120
3	Target-Based Evaluation of â€œDrug-Likeâ€•Properties and Ligand Efficiencies. Journal of Medicinal Chemistry, 2021, 64, 7210-7230.	2.9	46
4	Validation of lipid-related therapeutic targets for coronary heart disease prevention using human genetics. Nature Communications, 2021, 12, 6120.	5.8	13
5	An open source chemical structure curation pipeline using RDKit. Journal of Cheminformatics, 2020, 12, 51.	2.8	166
6	The Global Phosphorylation Landscape of SARS-CoV-2 Infection. Cell, 2020, 182, 685-712.e19.	13.5	825
7	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.	2.8	4
8	Improving the odds of drug development success through human genomics: modelling study. Scientific Reports, 2019, 9, 18911.	1.6	112
9	ChEMBL: towards direct deposition of bioassay data. Nucleic Acids Research, 2019, 47, D930-D940.	6.5	1,212
10	Large scale comparison of QSAR and conformal prediction methods and their applications in drug discovery. Journal of Cheminformatics, 2019, 11, 4.	2.8	93
11	Unexplored therapeutic opportunities in the human genome. Nature Reviews Drug Discovery, 2018, 17, 317-332.	21.5	263
12	A large-scale dataset of in vivo pharmacology assay results. Scientific Data, 2018, 5, 180230.	2.4	8
13	Pharos: Collating protein information to shed light on the druggable genome. Nucleic Acids Research, 2017, 45, D995-D1002.	6.5	271
14	A comprehensive map of molecular drug targets. Nature Reviews Drug Discovery, 2017, 16, 19-34.	21.5	1,608
15	The druggable genome and support for target identification and validation in drug development. Science Translational Medicine, 2017, 9, .	5.8	437
16	Open Targets: a platform for therapeutic target identification and validation. Nucleic Acids Research, 2017, 45, D985-D994.	6.5	355
17	The ChEMBL database in 2017. Nucleic Acids Research, 2017, 45, D945-D954.	6.5	1,718
18	Using ChEMBL web services for building applications and data processing workflows relevant to drug discovery. Expert Opinion on Drug Discovery, 2017, 12, 757-767.	2.5	24

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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.	0.9	27
20	SureChEMBL: a large-scale, chemically annotated patent document database. Nucleic Acids Research, 2016, 44, D1220-D1228.	6.5	156
21	A large-scale crop protection bioassay data set. Scientific Data, 2015, 2, 150032.	2.4	18
22	Managing expectations: assessment of chemistry databases generated by automated extraction of chemical structures from patents. Journal of Cheminformatics, 2015, 7, 49.	2.8	19
23	ChEMBL web services: streamlining access to drug discovery data and utilities. Nucleic Acids Research, 2015, 43, W612-W620.	6.5	437
24	The complex portal - an encyclopaedia of macromolecular complexes. Nucleic Acids Research, 2015, 43, D479-D484.	6.5	100
25	PPDMsâ€"a resource for mapping small molecule bioactivities from ChEMBL to Pfam-A protein domains. Bioinformatics, 2015, 31, 776-778.	1.8	11
26	Chemical databases: curation or integration by user-defined equivalence?. Drug Discovery Today: Technologies, 2015, 14, 17-24.	4.0	43
27	Activity, assay and target data curation and quality in the ChEMBL database. Journal of Computer-Aided Molecular Design, 2015, 29, 885-896.	1.3	118
28	The ChEMBL bioactivity database: an update. Nucleic Acids Research, 2014, 42, D1083-D1090.	6.5	1,283
29	Chemical, Target, and Bioactive Properties of Allosteric Modulation. PLoS Computational Biology, 2014, 10, e1003559.	1.5	75
30	The EBI RDF platform: linked open data for the life sciences. Bioinformatics, 2014, 30, 1338-1339.	1.8	190
31	UniChem: extension of InChI-based compound mapping to salt, connectivity and stereochemistry layers. Journal of Cheminformatics, 2014, 6, 43.	2.8	28
32	Transporter taxonomy â€“ a comparison of different transport protein classification schemes. Drug Discovery Today: Technologies, 2014, 12, e37-e46.	4.0	7
33	Transporter assays and assay ontologies: useful tools for drug discovery. Drug Discovery Today: Technologies, 2014, 12, e47-e54.	4.0	4
34	Scientific Lenses to Support Multiple Views over Linked Chemistry Data. Lecture Notes in Computer Science, 2014, , 98-113.	1.0	16
35	UniChem: a unified chemical structure cross-referencing and identifier tracking system. Journal of Cheminformatics, 2013, 5, 3.	2.8	133
36	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.	21.5	0

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37	ChEMBL: a large-scale bioactivity database for drug discovery. Nucleic Acids Research, 2012, 40, D1100-D1107.	6.5	3,028
38	PSICQUIC and PSISCORE: accessing and scoring molecular interactions. Nature Methods, 2011, 8, 528-529.	9.0	274
39	Minimum information about a bioactive entity (MIABE). Nature Reviews Drug Discovery, 2011, 10, 661-669.	21.5	80
40	Collation and data-mining of literature bioactivity data for drug discovery. Biochemical Society Transactions, 2011, 39, 1365-1370.	1.6	31
41	Visualizing the drug target landscape. Drug Discovery Today, 2010, 15, 3-15.	3.2	50
42	Role of open chemical data in aiding drug discovery and design. Future Medicinal Chemistry, 2010, 2, 903-907.	1.1	20
43	Drug target central. Expert Opinion on Drug Discovery, 2009, 4, 857-872.	2.5	16
44	Functional assignment of MAPK phosphatase domains. Proteins: Structure, Function and Bioinformatics, 2007, 69, 19-31.	1.5	12
45	The PRINTS protein fingerprint database: functional and evolutionary applications. , 2006, , .		2
46	The PRINTS protein fingerprint database: functional and evolutionary applications. , 2005, , .		1
47	Bioinformatics approaches for the classification of G-protein-coupled receptors. Current Opinion in Pharmacology, 2003, 3, 114-120.	1.7	38
48	Motif3D: relating protein sequence motifs to 3D structure. Nucleic Acids Research, 2003, 31, 3333-3336.	6.5	11
49	The Molecular Basis of Predicting Druggability. , 0, , 1315-1334.		5