Andrew R Leach

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1522428/publications.pdf

Version: 2024-02-01

77 papers	16,720 citations	117625 34 h-index	85541 71 g-index
96 all docs	96 docs citations	96 times ranked	19854 citing authors

#	Article	IF	Citations
1	Development and validation of a genetic algorithm for flexible docking 1 1Edited by F. E. Cohen. Journal of Molecular Biology, 1997, 267, 727-748.	4.2	5,937
2	The ChEMBL database in 2017. Nucleic Acids Research, 2017, 45, D945-D954.	14.5	1,718
3	ChEMBL: towards direct deposition of bioassay data. Nucleic Acids Research, 2019, 47, D930-D940.	14.5	1,212
4	An analysis of the attrition of drug candidates from four major pharmaceutical companies. Nature Reviews Drug Discovery, 2015, 14, 475-486.	46.4	996
5	Molecular Complexity and Its Impact on the Probability of Finding Leads for Drug Discovery. Journal of Chemical Information and Computer Sciences, 2001, 41, 856-864.	2.8	865
6	The Global Phosphorylation Landscape of SARS-CoV-2 Infection. Cell, 2020, 182, 685-712.e19.	28.9	825
7	Prediction of Proteinâ^'Ligand Interactions. Docking and Scoring:Â Successes and Gaps. Journal of Medicinal Chemistry, 2006, 49, 5851-5855.	6.4	603
8	Ligand docking to proteins with discrete side-chain flexibility. Journal of Molecular Biology, 1994, 235, 345-356.	4.2	344
9	Three-Dimensional Pharmacophore Methods in Drug Discovery. Journal of Medicinal Chemistry, 2010, 53, 539-558.	6.4	326
10	Unexplored therapeutic opportunities in the human genome. Nature Reviews Drug Discovery, 2018, 17, 317-332.	46.4	263
11	An Introduction To Chemoinformatics. , 2007, , .		259
12	Ligand solvation in molecular docking. Proteins: Structure, Function and Bioinformatics, 1999, 34, 4-16.	2.6	252
13	Conformational analysis of flexible ligands in macromolecular receptor sites. Journal of Computational Chemistry, 1992, 13, 730-748.	3.3	201
14	Exploring the conformational space of protein side chains using dead-end elimination and the A* algorithm. Proteins: Structure, Function and Bioinformatics, 1998, 33, 227-239.	2.6	187
15	An open source chemical structure curation pipeline using RDKit. Journal of Cheminformatics, 2020, 12, 51.	6.1	166
16	Molecular complexity and fragment-based drug discovery: ten years on. Current Opinion in Chemical Biology, 2011, 15, 489-496.	6.1	152
17	Fragment screening: an introduction. Molecular BioSystems, 2006, 2, 429.	2.9	141
18	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

#	Article	IF	Citations
19	A comparison of the pharmacophore identification programs: Catalyst, DISCO and GASP. Journal of Computer-Aided Molecular Design, 2002, 16, 653-681.	2.9	123
20	Actionable druggable genome-wide Mendelian randomization identifies repurposing opportunities for COVID-19. Nature Medicine, 2021, 27, 668-676.	30.7	120
21	The in silico world of virtual libraries. Drug Discovery Today, 2000, 5, 326-336.	6.4	119
22	The PROTACtable genome. Nature Reviews Drug Discovery, 2021, 20, 789-797.	46.4	112
23	Prediction of Biological Activity for High-Throughput Screening Using Binary Kernel Discrimination. Journal of Chemical Information and Computer Sciences, 2001, 41, 1295-1300.	2.8	110
24	Large scale comparison of QSAR and conformal prediction methods and their applications in drug discovery. Journal of Cheminformatics, 2019, 11, 4.	6.1	93
25	Implementation of a System for Reagent Selection and Library Enumeration, Profiling, and Designâ€. Journal of Chemical Information and Computer Sciences, 1999, 39, 1161-1172.	2.8	90
26	Binding Constants of Neuraminidase Inhibitors:Â An Investigation of the Linear Interaction Energy Method. Journal of Medicinal Chemistry, 1999, 42, 5142-5152.	6.4	81
27	WIZARD: AI in conformational analysis. Journal of Computer-Aided Molecular Design, 1987, 1, 73-85.	2.9	73
28	Drug mechanismâ€•ofâ€•action discovery through the integration of pharmacological and <scp>CRISPR</scp> screens. Molecular Systems Biology, 2020, 16, e9405.	7.2	63
29	Current methods for site-directed structure generation. Journal of Computer-Aided Molecular Design, 1994, 8, 467-475.	2.9	58
30	A Comparison of Field-Based Similarity Searching Methods: CatShape, FBSS, and ROCS. Journal of Chemical Information and Modeling, 2008, 48, 719-729.	5.4	57
31	Automated conformational analysis: Directed conformational search using the A* algorithm. Journal of Computational Chemistry, 1990, 11, 1193-1205.	3.3	56
32	A Survey of Methods for Searching the Conformational Space of Small and Medium-Sized Molecules. Reviews in Computational Chemistry, 2007, , 1-55.	1.5	54
33	The ELIXIR Core Data Resources: fundamental infrastructure for the life sciences. Bioinformatics, 2020, 36, 2636-2642.	4.1	47
34	Target-Based Evaluation of â€œDrug-Likeâ€•Properties and Ligand Efficiencies. Journal of Medicinal Chemistry, 2021, 64, 7210-7230.	6.4	46
35	Target 2035 â€“ update on the quest for a probe for every protein. RSC Medicinal Chemistry, 2022, 13, 13-21.	3.9	39
36	Theoretical investigations of novel nucleic acid bases. Journal of the American Chemical Society, 1992, 114, 3675-3683.	13.7	38

#	Article	IF	Citations
37	The application of Artificial Intelligence to the conformational analysis of strained molecules. Journal of Computational Chemistry, 1990, 11, 680-693.	3.3	33
38	Automated conformational analysis and structure generation: algorithms for molecular perception. Journal of Chemical Information and Modeling, 1990, 30, 316-324.	5.4	31
39	Synergy between combinatorial chemistry and de novo design22European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, Cambridge CB10 1SD, United Kingdom.. Journal of Molecular Graphics and Modelling, 2000, 18, 358-367.	2.4	30
40	Design and synthesis of orally active pyrrolidin-2-one-based factor Xa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 3784-3788.	2.2	30
41	Analysis and optimization of structure-based virtual screening protocols. Journal of Molecular Graphics and Modelling, 2003, 22, 41-53.	2.4	29
42	Automated molecular design: A new fragment-joining algorithm. Journal of Computer-Aided Molecular Design, 1994, 8, 283-298.	2.9	27
43	PLUMS:â€‰a Program for the Rapid Optimization of Focused Libraries. Journal of Chemical Information and Computer Sciences, 2000, 40, 1441-1448.	2.8	27
44	Where Are the GaPs? A Rational Approach to Monomer Acquisition and Selectionâ€. Journal of Chemical Information and Computer Sciences, 2000, 40, 1262-1269.	2.8	26
45	An investigation into the construction of molecular models by the template joining method. Journal of Computer-Aided Molecular Design, 1988, 2, 107-123.	2.9	25
46	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
47	Automated conformational analysis: Algorithms for the efficient construction of low-energy conformations. Journal of Computer-Aided Molecular Design, 1990, 4, 271-282.	2.9	23
48	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
49	A combined model-building and distance-geometry approach to automated conformational analysis and search. Journal of Chemical Information and Computer Sciences, 1992, 32, 379-385.	2.8	21
50	Further Development of a Genetic Algorithm for Ligand Docking and Its Application to Screening Combinatorial Libraries. ACS Symposium Series, 1999, , 271-291.	0.5	20
51	MAIP: a web service for predicting bloodâ€stage malaria inhibitors. Journal of Cheminformatics, 2021, 13, 13.	6.1	20
52	EnantioselectiveN-oxygenation of chlorpheniramine by the flavin-containing monooxygenase from hog liver. Xenobiotica, 1992, 22, 459-469.	1.1	19
53	An Algorithm To Directly Identify a Molecule's "Most Different" Conformations. Journal of Chemical Information and Computer Sciences, 1994, 34, 661-670.	2.8	18
54	A ring-bracing approach to computer-assisted ligand design. Journal of Computational Chemistry, 1994, 15, 233-240.	3.3	16

#	Article	IF	Citations
55	Hotspots API: A Python Package for the Detection of Small Molecule Binding Hotspots and Application to Structure-Based Drug Design. Journal of Chemical Information and Modeling, 2020, 60, 1911-1916.	5.4	15
56	Drug Safety Data Curation and Modeling in ChEMBL: Boxed Warnings and Withdrawn Drugs. Chemical Research in Toxicology, 2021, 34, 385-395.	3.3	15
57	Synthesis and solution conformation of a C2 symmetric macrobicycle. Tetrahedron Letters, 1995, 36, 3047-3050.	1.4	12
58	The Application of Neural Networks in Conformational Analysis. 1. Prediction of Minimum and Maximum Interatomic Distances. Journal of Chemical Information and Computer Sciences, 1995, 35, 640-650.	2.8	12
59	Computer-aided molecular design under the SWOTlight. Journal of Computer-Aided Molecular Design, 2012, 26, 51-56.	2.9	11
60	A molecular dynamics study of the inhibition of chicken dihydrofolate reductase by a phenyl triazine. Journal of Computational Chemistry, 1995, 16, 1378-1393.	3.3	9
61	The aggregation behaviour of two structurally isomeric glycolipids. Chemistry and Physics of Lipids, 1994, 74, 83-91.	3.2	8
62	Structure-based selection of building blocks for array synthesis via the World-Wide Web. Journal of Molecular Graphics and Modelling, 1997, 15, 158-160.	2.4	8
63	A large-scale dataset of in vivo pharmacology assay results. Scientific Data, 2018, 5, 180230.	5.3	8
64	Influence of HLA Class II Polymorphism on Predicted Cellular Immunity Against SARS-CoV-2 at the Population and Individual Level. Frontiers in Immunology, 2021, 12, 669357.	4.8	7
65	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
66	Displaying functions of three variables. Journal of Molecular Graphics, 1988, 6, 54-60.	1.1	3
67	Automated conformational analysis and structure generation. Pest Management Science, 1991, 33, 87-96.	0.4	3
68	Constitutional, configurational and conformational analysis of transition metal coordination complexes. Journal of Computer-Aided Molecular Design, 1993, 7, 225-240.	2.9	3
69	SAR Knowledge Bases in Drug Discovery. Annual Reports in Computational Chemistry, 2008, 4, 203-216.	1.7	2
70	The Enzyme Portal: an integrative tool for enzyme information and analysis. FEBS Journal, 2021, , .	4.7	2
71	Introduction to Fragment Screening. , 2007, , 49-72.		2
72	Computational Drug Target Tractability Analysis. , 2021, , 145-153.		1

#	Article	IF	Citations
73	Ligand solvation in molecular docking. , 1999, 34, 4.		1
74	Computational Chemistry in Lead Identification, Library Design and Lead Optimisation. Molecular Simulation, 2001, 26, 33-49.	2.0	0
75	Cheminformatics and computational chemistry in lead optimisation. Journal of Cheminformatics, 2011, 3, .	6.1	0
76	Reprint of: Characterising hepatic mitochondrial function as a model for systemic toxicity: A commentary. Toxicology, 2012, 302, e1-e4.	4.2	0
77	Characterising hepatic mitochondrial function as a model for systemic toxicity: A commentary. Toxicology, 2012, 302, 96-99.	4.2	0