Andrew R Leach

List of Publications by Year in Descending Order

80 papers	12,342 citations	32 h-index	96 g-index
96 ext. papers	14,608 ext. citations	10.5 avg, IF	6.12 L-index

#	Paper	IF	Citations
80	CACHE (Critical Assessment of Computational Hit-finding Experiments): A public–private partnership benchmarking initiative to enable the development of computational methods for hit-finding. *Nature Reviews Chemistry*, **2022**, 6, 287-295	34.6	1
79	Actionable druggable genome-wide Mendelian randomization identifies repurposing opportunities for COVID-19. *Nature Medicine*, **2021**, 27, 668-676	50.5	19
78	Target-Based Evaluation of "Drug-Like" Properties and Ligand Efficiencies. *Journal of Medicinal Chemistry*, **2021**, 64, 7210-7230	8.3	9
77	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	8.4	3
76	Drug Safety Data Curation and Modeling in ChEMBL: Boxed Warnings and Withdrawn Drugs. *Chemical Research in Toxicology*, **2021**, 34, 385-395	4	3
75	Computational Drug Target Tractability Analysis **2021**, 145-153		0
74	MAIP: a web service for predicting blood-stage malaria inhibitors. *Journal of Cheminformatics*, **2021**, 13, 13	8.6	3
73	The PROTACtable genome. *Nature Reviews Drug Discovery*, **2021**, 20, 789-797	64.1	20
72	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	6.1	8
71	The Global Phosphorylation Landscape of SARS-CoV-2 Infection. *Cell*, **2020**, 182, 685-712.e19	56.2	439
70	The ELIXIR Core Data Resources: fundamental infrastructure for the life sciences. *Bioinformatics*, **2020**, 36, 2636-2642	7.2	29
69	Drug mechanism-of-action discovery through the integration of pharmacological and CRISPR screens. *Molecular Systems Biology*, **2020**, 16, e9405	12.2	22
68	An open source chemical structure curation pipeline using RDKit. *Journal of Cheminformatics*, **2020**, 12, 51	8.6	40
67	Reply to "Missed opportunities in large scale comparison of QSAR and conformal prediction methods and their applications in drug discovery". *Journal of Cheminformatics*, **2019**, 11, 64	8.6	2
66	ChEMBL: towards direct deposition of bioassay data. *Nucleic Acids Research*, **2019**, 47, D930-D940	20.1	453
65	Large scale comparison of QSAR and conformal prediction methods and their applications in drug discovery. *Journal of Cheminformatics*, **2019**, 11, 4	8.6	53
64	Unexplored therapeutic opportunities in the human genome. *Nature Reviews Drug Discovery*, **2018**, 17, 317-332	64.1	156

63	Drug Target Commons: A Community Effort to Build a Consensus Knowledge Base for Drug-Target Interactions. *Cell Chemical Biology*, **2018**, 25, 224-229.e2	8.2	51
62	A large-scale dataset of in vivo pharmacology assay results. *Scientific Data*, **2018**, 5, 180230	8.2	6
61	The ChEMBL database in 2017. *Nucleic Acids Research*, **2017**, 45, D945-D954	20.1	1059
60	Using ChEMBL web services for building applications and data processing workflows relevant to drug discovery. *Expert Opinion on Drug Discovery*, **2017**, 12, 757-767	6.2	12
59	An analysis of the attrition of drug candidates from four major pharmaceutical companies. *Nature Reviews Drug Discovery*, **2015**, 14, 475-86	64.1	713
58	Coping with Complexity in Molecular Design **2013**, 57-77		1
57	Computer-aided molecular design under the SWOTlight. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 51-6	4.2	11
56	Reprint of: Characterising hepatic mitochondrial function as a model for systemic toxicity: a commentary. *Toxicology*, **2012**, 302, e1-4	4.4	
55	Cheminformatics and computational chemistry in lead optimisation. *Journal of Cheminformatics*, **2011**, 3,	8.6	78
54	Molecular complexity and fragment-based drug discovery: ten years on. *Current Opinion in Chemical Biology*, **2011**, 15, 489-96	9.7	129
53	Three-dimensional pharmacophore methods in drug discovery. *Journal of Medicinal Chemistry*, **2010** , 53, 539-58	8.3	283
52	SAR Knowledge Bases in Drug Discovery. *Annual Reports in Computational Chemistry*, **2008**, 4, 203-216	1.8	2
51	A comparison of field-based similarity searching methods: CatShape, FBSS, and ROCS. *Journal of Chemical Information and Modeling*, **2008**, 48, 719-29	6.1	52
50	An Introduction To Chemoinformatics **2007**,		191
49	Structure-Based Drug Discovery **2007**,		23
48	A Survey of Methods for Searching the Conformational Space of Small and Medium-Sized Molecules. *Reviews in Computational Chemistry*, **2007**, 1-55		35
47	Introduction to Fragment Screening **2007**, 49-72		1
46	Prediction of protein-ligand interactions. Docking and scoring: successes and gaps. *Journal of Medicinal Chemistry*, **2006**, 49, 5851-5	8.3	542

45	Fragment screening: an introduction. *Molecular BioSystems*, **2006**, 2, 430-46		123
44	Design and synthesis of orally active pyrrolidin-2-one-based factor Xa inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 3784-8	2.9	27
43	Computational Chemistry, Molecular Complexity and Screening Set Design. *Methods and Principles in Medicinal Chemistry*, **2005**, 43-57	0.4	4
42	Analysis and optimization of structure-based virtual screening protocols. (3). New methods and old problems in scoring function design. *Journal of Molecular Graphics and Modelling*, **2003**, 22, 41-53	2.8	29
41	A comparison of the pharmacophore identification programs: Catalyst, DISCO and GASP. *Journal of Computer-Aided Molecular Design*, **2002**, 16, 653-81	4.2	106
40	Computational Chemistry in Lead Identification, Library Design and Lead Optimisation. *Molecular Simulation*, **2001**, 26, 33-49	2	
39	Molecular complexity and its impact on the probability of finding leads for drug discovery. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 856-64		761
38	Prediction of biological activity for high-throughput screening using binary kernel discrimination. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1295-300		97
37	Synergy between combinatorial chemistry and de novo design. *Journal of Molecular Graphics and Modelling*, **2000**, 18, 358-67, 526	2.8	22
36	The in silico world of virtual libraries. *Drug Discovery Today*, **2000**, 5, 326-336	8.8	109
35	Where are the GaPs? A rational approach to monomer acquisition and selection. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 1262-9		25
34	PLUMS: a program for the rapid optimization of focused libraries. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 1441-8		23
33	Ligand solvation in molecular docking. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 4-16	4.2	223
32	Binding constants of neuraminidase inhibitors: An investigation of the linear interaction energy method. *Journal of Medicinal Chemistry*, **1999**, 42, 5142-52	8.3	77
31	Implementation of a system for reagent selection and library enumeration, profiling, and design. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 1161-72		80
30	Further Development of a Genetic Algorithm for Ligand Docking and Its Application to Screening Combinatorial Libraries. *ACS Symposium Series*, **1999**, 271-291	0.4	14
29	Ligand solvation in molecular docking **1999**, 34, 4		1
28	Exploring the conformational space of protein side chains using dead-end elimination and the A* algorithm. *Proteins: Structure, Function and Bioinformatics*, **1998**, 33, 227-39	4.2	167

27	Development and validation of a genetic algorithm for flexible docking. *Journal of Molecular Biology*, **1997**, 267, 727-48	6.5	5041
26	Structure-based selection of building blocks for array synthesis via the World-Wide Web. *Journal of Molecular Graphics and Modelling*, **1997**, 15, 158-60, 180	2.8	7
25	Synthesis and solution conformation of a C2 symmetric macrobicycle. *Tetrahedron Letters*, **1995**, 36, 3047-3050	2	10
24	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		7
23	A molecular dynamics study of the inhibition of chicken dihydrofolate reductase by a phenyl triazine. *Journal of Computational Chemistry*, **1995**, 16, 1378-1393	3.5	7
22	Current methods for site-directed structure generation. *Journal of Computer-Aided Molecular Design*, **1994**, 8, 467-75	4.2	48
21	Automated molecular design: a new fragment-joining algorithm. *Journal of Computer-Aided Molecular Design*, **1994**, 8, 283-98	4.2	26
20	The aggregation behaviour of two structurally isomeric glycolipids. *Chemistry and Physics of Lipids*, **1994**, 74, 83-91	3.7	8
19	A ring-bracing approach to computer-assisted ligand design. *Journal of Computational Chemistry*, **1994**, 15, 233-240	3.5	15
18	Ligand docking to proteins with discrete side-chain flexibility. *Journal of Molecular Biology*, **1994**, 235, 345-56	6.5	314
17	An Algorithm To Directly Identify a Molecule's "Most Different" Conformations. *Journal of Chemical Information and Computer Sciences*, **1994**, 34, 661-670		14
16	Applications of Artificial Intelligence in Molecular Modelling and Drug Design **1994**, 211-265		
15	Constitutional, configurational and conformational analysis of transition metal coordination complexes. *Journal of Computer-Aided Molecular Design*, **1993**, 7, 225-40	4.2	2
14	Enantioselective N-oxygenation of chlorpheniramine by the flavin-containing monooxygenase from hog liver. *Xenobiotica*, **1992**, 22, 459-69	2	16
13	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		18
12	Theoretical investigations of novel nucleic acid bases. *Journal of the American Chemical Society*, **1992**, 114, 3675-3683	16.4	36
11	Conformational analysis of flexible ligands in macromolecular receptor sites. *Journal of Computational Chemistry*, **1992**, 13, 730-748	3.5	171
10	Automated conformational analysis and structure generation. *Pest Management Science*, **1991**, 33, 87-96		3

9	Automated conformational analysis: algorithms for the efficient construction of low-energy conformations. *Journal of Computer-Aided Molecular Design*, **1990**, 4, 271-82	4.2	19
8	The application of Artificial Intelligence to the conformational analysis of strained molecules. *Journal of Computational Chemistry*, **1990**, 11, 680-693	3.5	29
7	Automated conformational analysis: Directed conformational search using the A* algorithm. *Journal of Computational Chemistry*, **1990**, 11, 1193-1205	3.5	49
6	Automated conformational analysis and structure generation: algorithms for molecular perception. *Journal of Chemical Information and Modeling*, **1990**, 30, 316-24	6.1	28
5	An investigation into the construction of molecular models by the template joining method. *Journal of Computer-Aided Molecular Design*, **1988**, 2, 107-23	4.2	22
4	Displaying functions of three variables. *Journal of Molecular Graphics*, **1988**, 6, 54-60		3
3	WIZARD: AI in conformational analysis. *Journal of Computer-Aided Molecular Design*, **1987**, 1, 73-85	4.2	64
2	Actionable druggable genome-wide Mendelian randomization identifies repurposing opportunities for COVID-19		1
1	Artificial Intelligence in Medicinal Chemistry1-19		