

# Andrew R Leach

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Development and validation of a genetic algorithm for flexible docking. <i>Journal of Molecular Biology</i> , <b>1997</b> , 267, 727-48	6.5	5041
79	The ChEMBL database in 2017. <i>Nucleic Acids Research</i> , <b>2017</b> , 45, D945-D954	20.1	1059
78	Molecular complexity and its impact on the probability of finding leads for drug discovery. <i>Journal of Chemical Information and Computer Sciences</i> , <b>2001</b> , 41, 856-64		761
77	An analysis of the attrition of drug candidates from four major pharmaceutical companies. <i>Nature Reviews Drug Discovery</i> , <b>2015</b> , 14, 475-86	64.1	713
76	Prediction of protein-ligand interactions. Docking and scoring: successes and gaps. <i>Journal of Medicinal Chemistry</i> , <b>2006</b> , 49, 5851-5	8.3	542
75	ChEMBL: towards direct deposition of bioassay data. <i>Nucleic Acids Research</i> , <b>2019</b> , 47, D930-D940	20.1	453
74	The Global Phosphorylation Landscape of SARS-CoV-2 Infection. <i>Cell</i> , <b>2020</b> , 182, 685-712.e19	56.2	439
73	Ligand docking to proteins with discrete side-chain flexibility. <i>Journal of Molecular Biology</i> , <b>1994</b> , 235, 345-56	6.5	314
72	Three-dimensional pharmacophore methods in drug discovery. <i>Journal of Medicinal Chemistry</i> , <b>2010</b> , 53, 539-58	8.3	283
71	Ligand solvation in molecular docking. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1999</b> , 34, 4-16	4.2	223
70	An Introduction To Chemoinformatics <b>2007</b> ,		191
69	Conformational analysis of flexible ligands in macromolecular receptor sites. <i>Journal of Computational Chemistry</i> , <b>1992</b> , 13, 730-748	3.5	171
68	Exploring the conformational space of protein side chains using dead-end elimination and the A* algorithm. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1998</b> , 33, 227-39	4.2	167
67	Unexplored therapeutic opportunities in the human genome. <i>Nature Reviews Drug Discovery</i> , <b>2018</b> , 17, 317-332	64.1	156
66	Molecular complexity and fragment-based drug discovery: ten years on. <i>Current Opinion in Chemical Biology</i> , <b>2011</b> , 15, 489-96	9.7	129
65	Fragment screening: an introduction. <i>Molecular BioSystems</i> , <b>2006</b> , 2, 430-46		123
64	The in silico world of virtual libraries. <i>Drug Discovery Today</i> , <b>2000</b> , 5, 326-336	8.8	109

63	A comparison of the pharmacophore identification programs: Catalyst, DISCO and GASP. <i>Journal of Computer-Aided Molecular Design</i> , <b>2002</b> , 16, 653-81	4.2	106
62	Prediction of biological activity for high-throughput screening using binary kernel discrimination. <i>Journal of Chemical Information and Computer Sciences</i> , <b>2001</b> , 41, 1295-300		97
61	Implementation of a system for reagent selection and library enumeration, profiling, and design. <i>Journal of Chemical Information and Computer Sciences</i> , <b>1999</b> , 39, 1161-72		80
60	Cheminformatics and computational chemistry in lead optimisation. <i>Journal of Cheminformatics</i> , <b>2011</b> , 3,	8.6	78
59	Binding constants of neuraminidase inhibitors: An investigation of the linear interaction energy method. <i>Journal of Medicinal Chemistry</i> , <b>1999</b> , 42, 5142-52	8.3	77
58	WIZARD: AI in conformational analysis. <i>Journal of Computer-Aided Molecular Design</i> , <b>1987</b> , 1, 73-85	4.2	64
57	Large scale comparison of QSAR and conformal prediction methods and their applications in drug discovery. <i>Journal of Cheminformatics</i> , <b>2019</b> , 11, 4	8.6	53
56	A comparison of field-based similarity searching methods: CatShape, FBSS, and ROCS. <i>Journal of Chemical Information and Modeling</i> , <b>2008</b> , 48, 719-29	6.1	52
55	Drug Target Commons: A Community Effort to Build a Consensus Knowledge Base for Drug-Target Interactions. <i>Cell Chemical Biology</i> , <b>2018</b> , 25, 224-229.e2	8.2	51
54	Automated conformational analysis: Directed conformational search using the A* algorithm. <i>Journal of Computational Chemistry</i> , <b>1990</b> , 11, 1193-1205	3.5	49
53	Current methods for site-directed structure generation. <i>Journal of Computer-Aided Molecular Design</i> , <b>1994</b> , 8, 467-75	4.2	48
52	An open source chemical structure curation pipeline using RDKit. <i>Journal of Cheminformatics</i> , <b>2020</b> , 12, 51	8.6	40
51	Theoretical investigations of novel nucleic acid bases. <i>Journal of the American Chemical Society</i> , <b>1992</b> , 114, 3675-3683	16.4	36
50	A Survey of Methods for Searching the Conformational Space of Small and Medium-Sized Molecules. <i>Reviews in Computational Chemistry</i> , <b>2007</b> , 1-55		35
49	The ELIXIR Core Data Resources: fundamental infrastructure for the life sciences. <i>Bioinformatics</i> , <b>2020</b> , 36, 2636-2642	7.2	29
48	Analysis and optimization of structure-based virtual screening protocols. (3). New methods and old problems in scoring function design. <i>Journal of Molecular Graphics and Modelling</i> , <b>2003</b> , 22, 41-53	2.8	29
47	The application of Artificial Intelligence to the conformational analysis of strained molecules. <i>Journal of Computational Chemistry</i> , <b>1990</b> , 11, 680-693	3.5	29
46	Automated conformational analysis and structure generation: algorithms for molecular perception. <i>Journal of Chemical Information and Modeling</i> , <b>1990</b> , 30, 316-24	6.1	28

45	Design and synthesis of orally active pyrrolidin-2-one-based factor Xa inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2006</b> , 16, 3784-8	2.9	27
44	Automated molecular design: a new fragment-joining algorithm. <i>Journal of Computer-Aided Molecular Design</i> , <b>1994</b> , 8, 283-98	4.2	26
43	Where are the GaPs? A rational approach to monomer acquisition and selection. <i>Journal of Chemical Information and Computer Sciences</i> , <b>2000</b> , 40, 1262-9		25
42	Structure-Based Drug Discovery <b>2007</b> ,		23
41	PLUMS: a program for the rapid optimization of focused libraries. <i>Journal of Chemical Information and Computer Sciences</i> , <b>2000</b> , 40, 1441-8		23
40	Synergy between combinatorial chemistry and de novo design. <i>Journal of Molecular Graphics and Modelling</i> , <b>2000</b> , 18, 358-67, 526	2.8	22
39	An investigation into the construction of molecular models by the template joining method. <i>Journal of Computer-Aided Molecular Design</i> , <b>1988</b> , 2, 107-23	4.2	22
38	Drug mechanism-of-action discovery through the integration of pharmacological and CRISPR screens. <i>Molecular Systems Biology</i> , <b>2020</b> , 16, e9405	12.2	22
37	The PROTACTable genome. <i>Nature Reviews Drug Discovery</i> , <b>2021</b> , 20, 789-797	64.1	20
36	Automated conformational analysis: algorithms for the efficient construction of low-energy conformations. <i>Journal of Computer-Aided Molecular Design</i> , <b>1990</b> , 4, 271-82	4.2	19
35	Actionable druggable genome-wide Mendelian randomization identifies repurposing opportunities for COVID-19. <i>Nature Medicine</i> , <b>2021</b> , 27, 668-676	50.5	19
34	A combined model-building and distance-geometry approach to automated conformational analysis and search. <i>Journal of Chemical Information and Computer Sciences</i> , <b>1992</b> , 32, 379-385		18
33	Enantioselective N-oxygenation of chlorpheniramine by the flavin-containing monooxygenase from hog liver. <i>Xenobiotica</i> , <b>1992</b> , 22, 459-69	2	16
32	A ring-bracing approach to computer-assisted ligand design. <i>Journal of Computational Chemistry</i> , <b>1994</b> , 15, 233-240	3.5	15
31	Further Development of a Genetic Algorithm for Ligand Docking and Its Application to Screening Combinatorial Libraries. <i>ACS Symposium Series</i> , <b>1999</b> , 271-291	0.4	14
30	An Algorithm To Directly Identify a Molecule's "Most Different" Conformations. <i>Journal of Chemical Information and Computer Sciences</i> , <b>1994</b> , 34, 661-670		14
29	Using ChEMBL web services for building applications and data processing workflows relevant to drug discovery. <i>Expert Opinion on Drug Discovery</i> , <b>2017</b> , 12, 757-767	6.2	12
28	Computer-aided molecular design under the SWOTlight. <i>Journal of Computer-Aided Molecular Design</i> , <b>2012</b> , 26, 51-6	4.2	11

27	Synthesis and solution conformation of a C2 symmetric macrobicycle. <i>Tetrahedron Letters</i> , <b>1995</b> , 36, 3047-3050	10	
26	Target-Based Evaluation of "Drug-Like" Properties and Ligand Efficiencies. <i>Journal of Medicinal Chemistry</i> , <b>2021</b> , 64, 7210-7230	8.3	9
25	Hotspots API: A Python Package for the Detection of Small Molecule Binding Hotspots and Application to Structure-Based Drug Design. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 1911-1916	6.1	8
24	The aggregation behaviour of two structurally isomeric glycolipids. <i>Chemistry and Physics of Lipids</i> , <b>1994</b> , 74, 83-91	3.7	8
23	Structure-based selection of building blocks for array synthesis via the World-Wide Web. <i>Journal of Molecular Graphics and Modelling</i> , <b>1997</b> , 15, 158-60, 180	2.8	7
22	The Application of Neural Networks in Conformational Analysis. 1. Prediction of Minimum and Maximum Interatomic Distances. <i>Journal of Chemical Information and Computer Sciences</i> , <b>1995</b> , 35, 640-650		7
21	A molecular dynamics study of the inhibition of chicken dihydrofolate reductase by a phenyl triazine. <i>Journal of Computational Chemistry</i> , <b>1995</b> , 16, 1378-1393	3.5	7
20	A large-scale dataset of in vivo pharmacology assay results. <i>Scientific Data</i> , <b>2018</b> , 5, 180230	8.2	6
19	Computational Chemistry, Molecular Complexity and Screening Set Design. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2005</b> , 43-57	0.4	4
18	Automated conformational analysis and structure generation. <i>Pest Management Science</i> , <b>1991</b> , 33, 87-96		3
17	Displaying functions of three variables. <i>Journal of Molecular Graphics</i> , <b>1988</b> , 6, 54-60		3
16	Influence of HLA Class II Polymorphism on Predicted Cellular Immunity Against SARS-CoV-2 at the Population and Individual Level. <i>Frontiers in Immunology</i> , <b>2021</b> , 12, 669357	8.4	3
15	Drug Safety Data Curation and Modeling in ChEMBL: Boxed Warnings and Withdrawn Drugs. <i>Chemical Research in Toxicology</i> , <b>2021</b> , 34, 385-395	4	3
14	MAIP: a web service for predicting blood-stage malaria inhibitors. <i>Journal of Cheminformatics</i> , <b>2021</b> , 13, 13	8.6	3
13	Reply to "Missed opportunities in large scale comparison of QSAR and conformal prediction methods and their applications in drug discovery". <i>Journal of Cheminformatics</i> , <b>2019</b> , 11, 64	8.6	2
12	SAR Knowledge Bases in Drug Discovery. <i>Annual Reports in Computational Chemistry</i> , <b>2008</b> , 4, 203-216	1.8	2
11	Constitutional, configurational and conformational analysis of transition metal coordination complexes. <i>Journal of Computer-Aided Molecular Design</i> , <b>1993</b> , 7, 225-40	4.2	2
10	Coping with Complexity in Molecular Design <b>2013</b> , 57-77		1

9	Introduction to Fragment Screening <b>2007</b> , 49-72		1
8	Actionable druggable genome-wide Mendelian randomization identifies repurposing opportunities for COVID-19		1
7	Ligand solvation in molecular docking <b>1999</b> , 34, 4		1
6	CACHE (Critical Assessment of Computational Hit-finding Experiments): A public-private partnership benchmarking initiative to enable the development of computational methods for hit-finding. <i>Nature Reviews Chemistry</i> , <b>2022</b> , 6, 287-295	34.6	1
5	Computational Drug Target Tractability Analysis <b>2021</b> , 145-153		0
4	Reprint of: Characterising hepatic mitochondrial function as a model for systemic toxicity: a commentary. <i>Toxicology</i> , <b>2012</b> , 302, e1-4	4.4	
3	Computational Chemistry in Lead Identification, Library Design and Lead Optimisation. <i>Molecular Simulation</i> , <b>2001</b> , 26, 33-49		2
2	Applications of Artificial Intelligence in Molecular Modelling and Drug Design <b>1994</b> , 211-265		
1	Artificial Intelligence in Medicinal Chemistry1-19		